

Using Metal Substrate to Enhance the Reactivity of Graphene towards Diels-Alder Reaction

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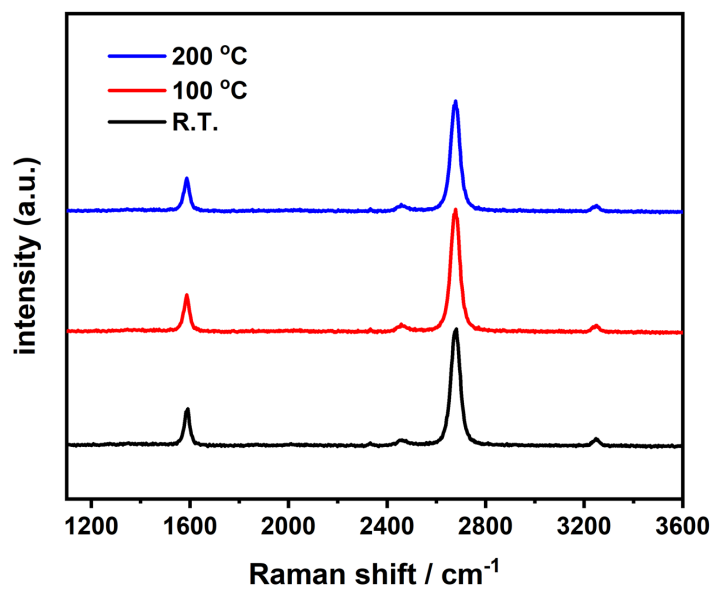


Figure S1. Raman spectra of graphene on silicon wafer casted with 10 μL xylenes followed by heating at room temperature (R.T., black), 100 $^{\circ}\text{C}$ (red), or 200 $^{\circ}\text{C}$ (blue) for 10 min.

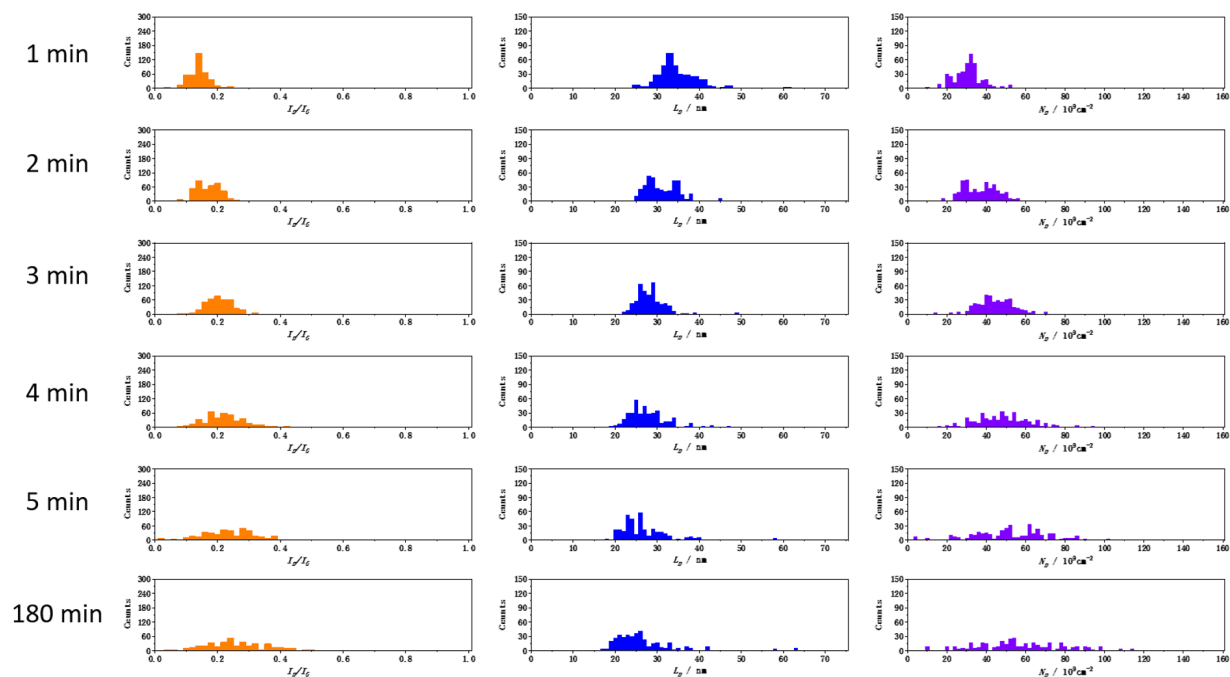


Figure S2. Histograms of (A) Raman I_D/I_G (B) L_D , and (C) n_D of G/SiO₂/Si after reacting with DMBD at 50 °C for different lengths of time. Results were from ~400 data points on 2 sets of independent samples.

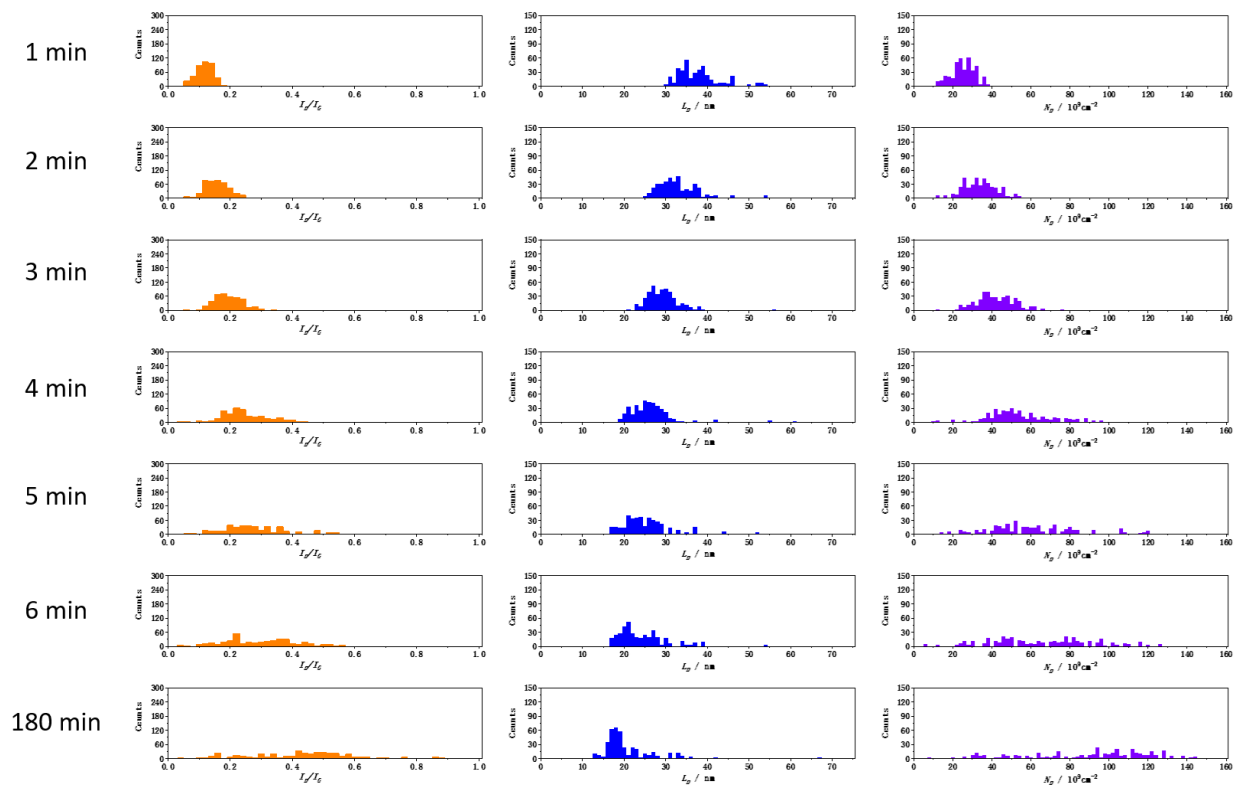


Figure S3. Histograms of (A) Raman I_D/I_G (B) L_D , and (C) n_D of G/Cu after reacting with DMBD at 50 °C for different lengths of time. Results were from ~400 data points on 2 sets of independent samples.

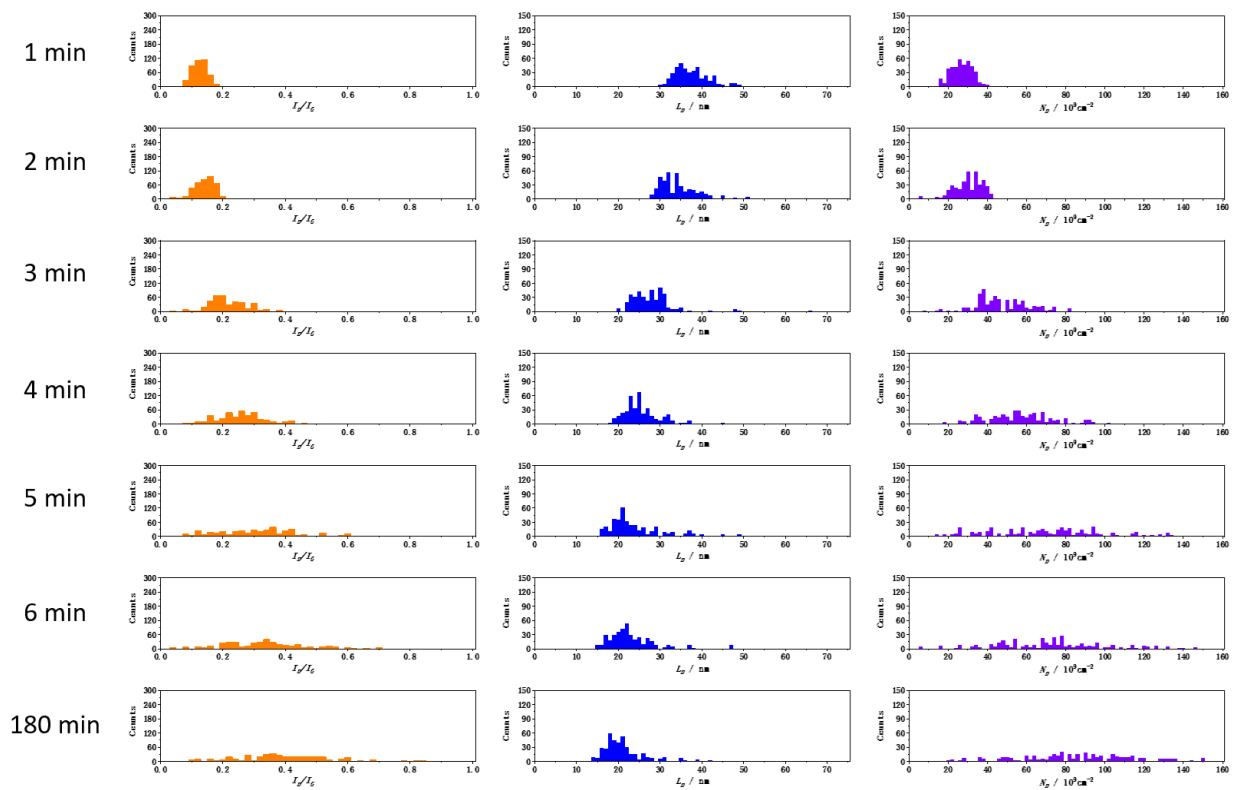


Figure S4. Histograms of (A) Raman I_D/I_G (B) L_D , and (C) n_D of G/Ni after reacting with DMBD at 50 °C for different lengths of time. Results were from ~400 data points on 2 sets of independent samples.

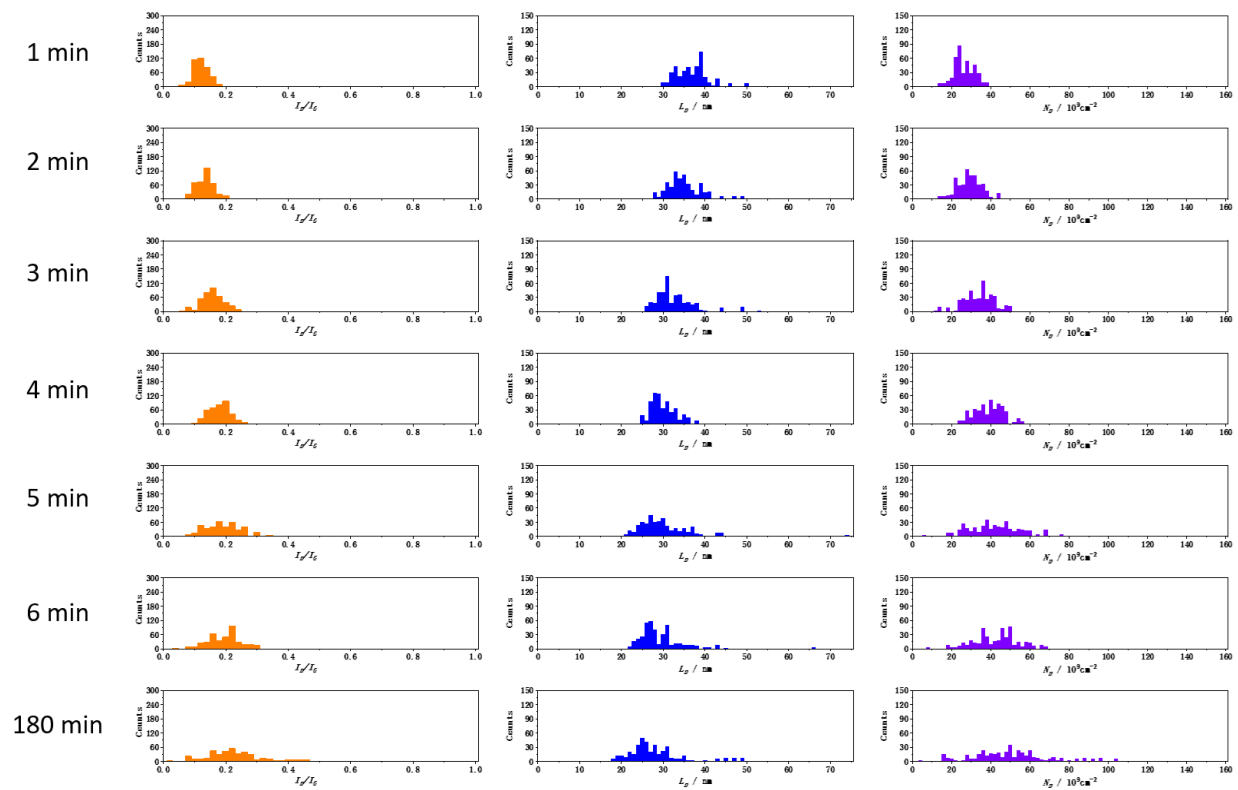


Figure S5. Histograms of (A) Raman I_D/I_G (B) L_D , and (C) n_D of G/SiO₂/Si after reacting with DMBD at 100 °C for different lengths of time. Results were from ~400 data points on 2 sets of independent samples.

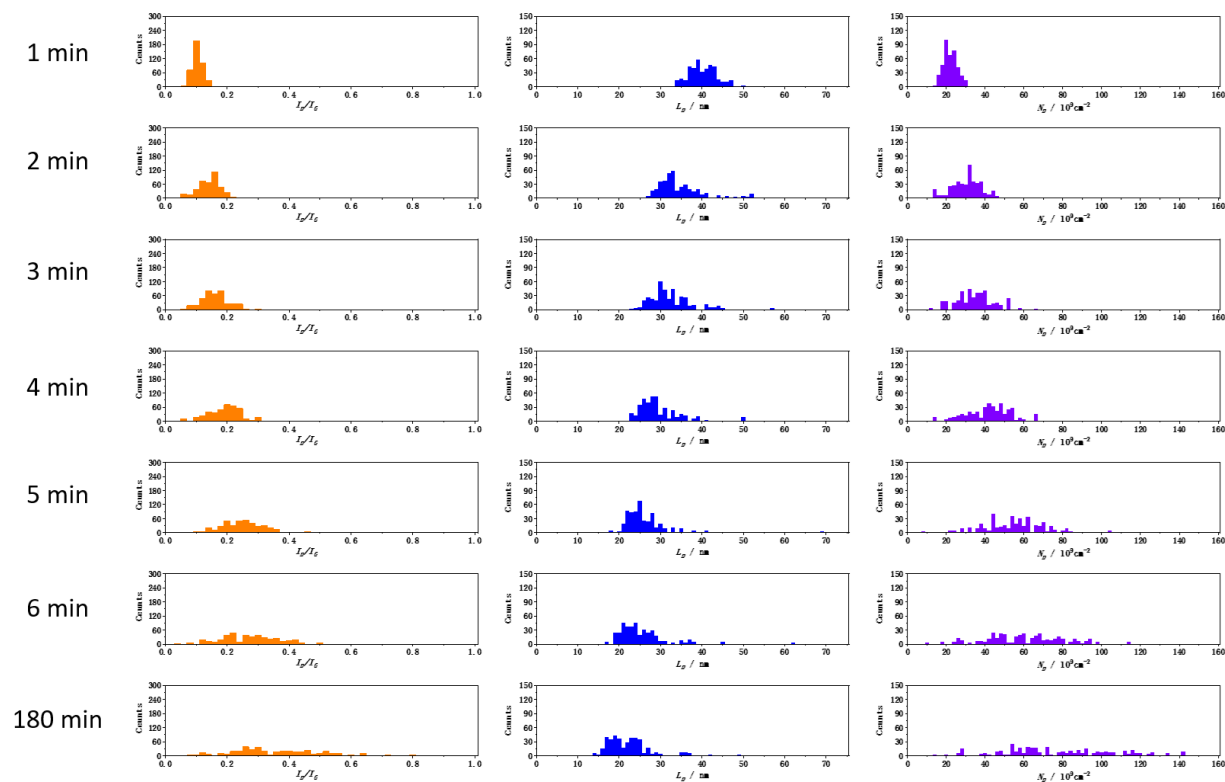


Figure S6. Histograms of (A) Raman I_D/I_G (B) L_D , and (C) n_D of G/Cu after reacting with DMBD at 100 °C for different lengths of time. Results were from ~ 400 data points on 2 sets of independent samples.

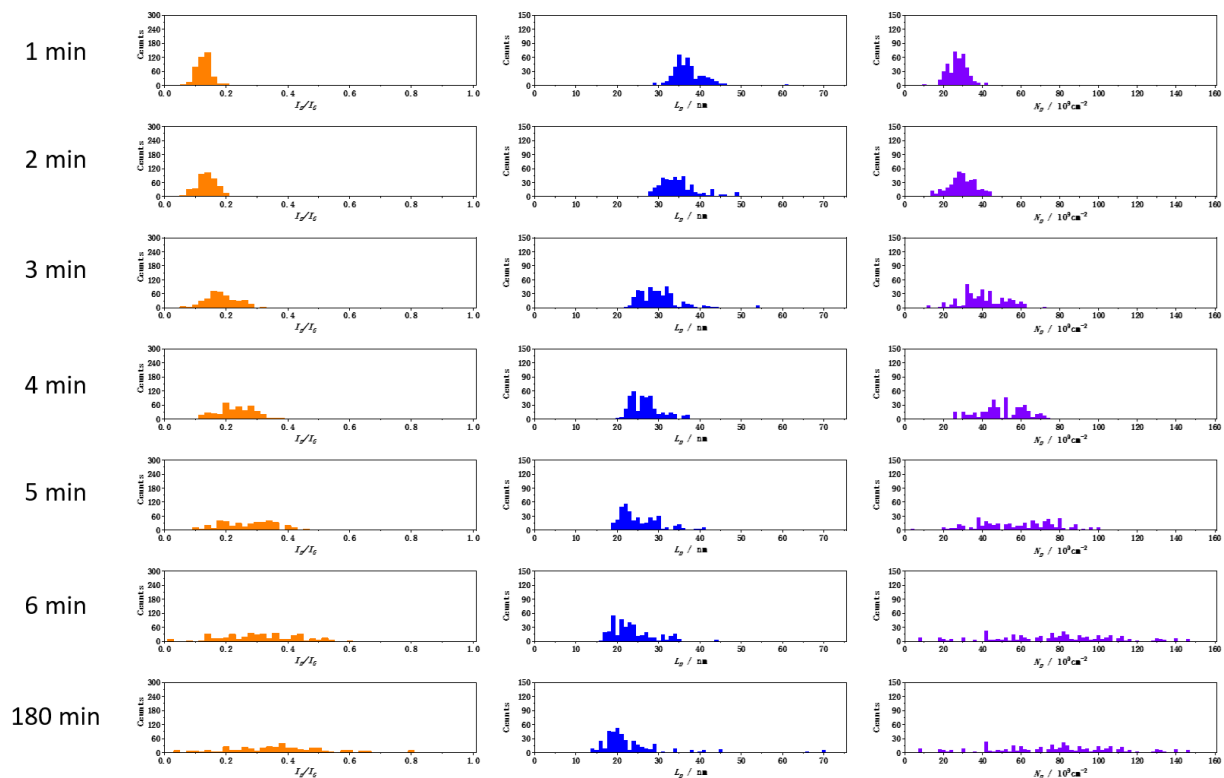


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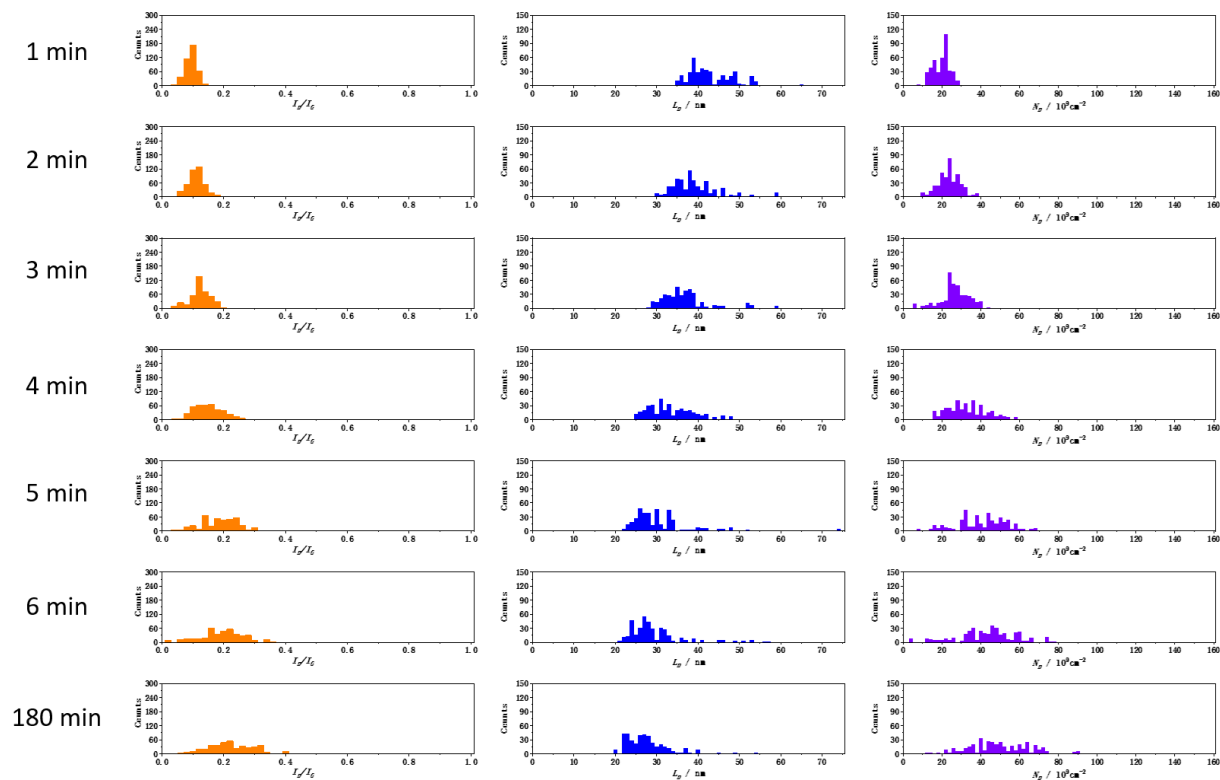


Figure S8. Histograms of (A) Raman I_D/I_G (B) L_D , and (C) n_D of G/SiO₂/Si after reacting with DMBD at 150 °C for different lengths of time. Results were from ~400 data points on 2 sets of independent samples.

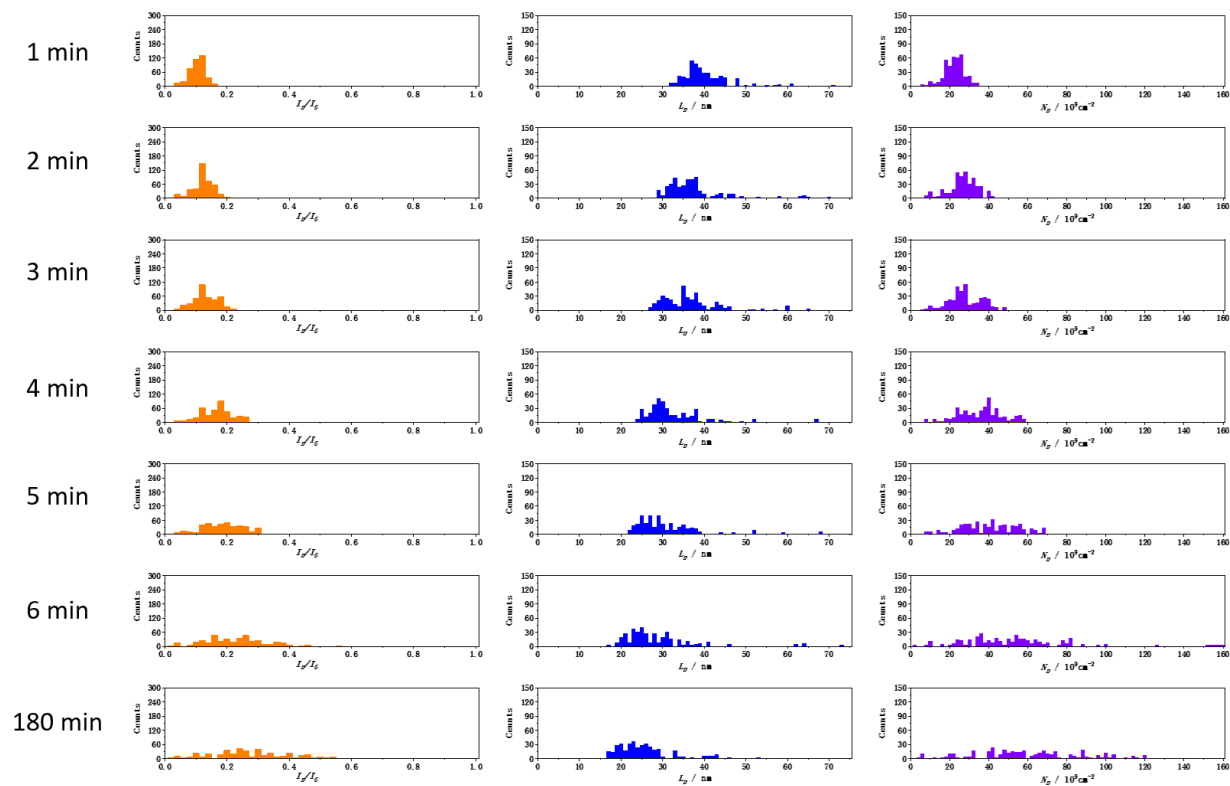


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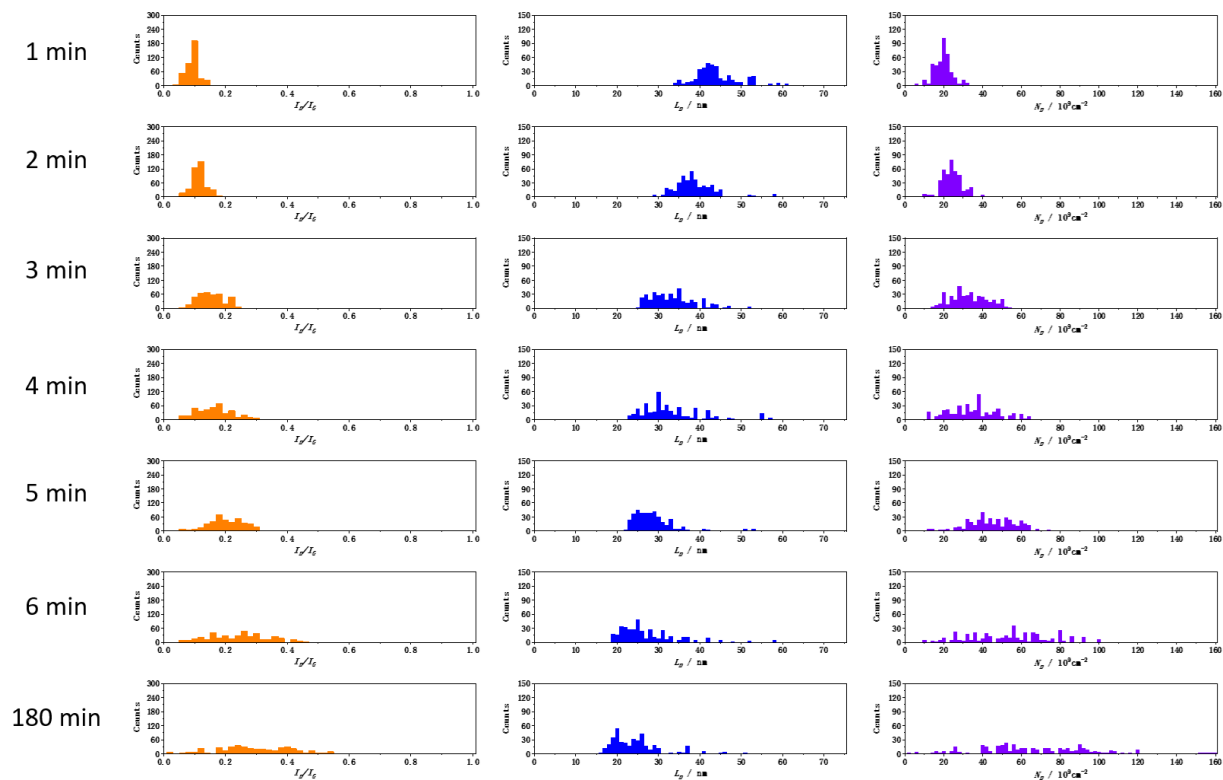


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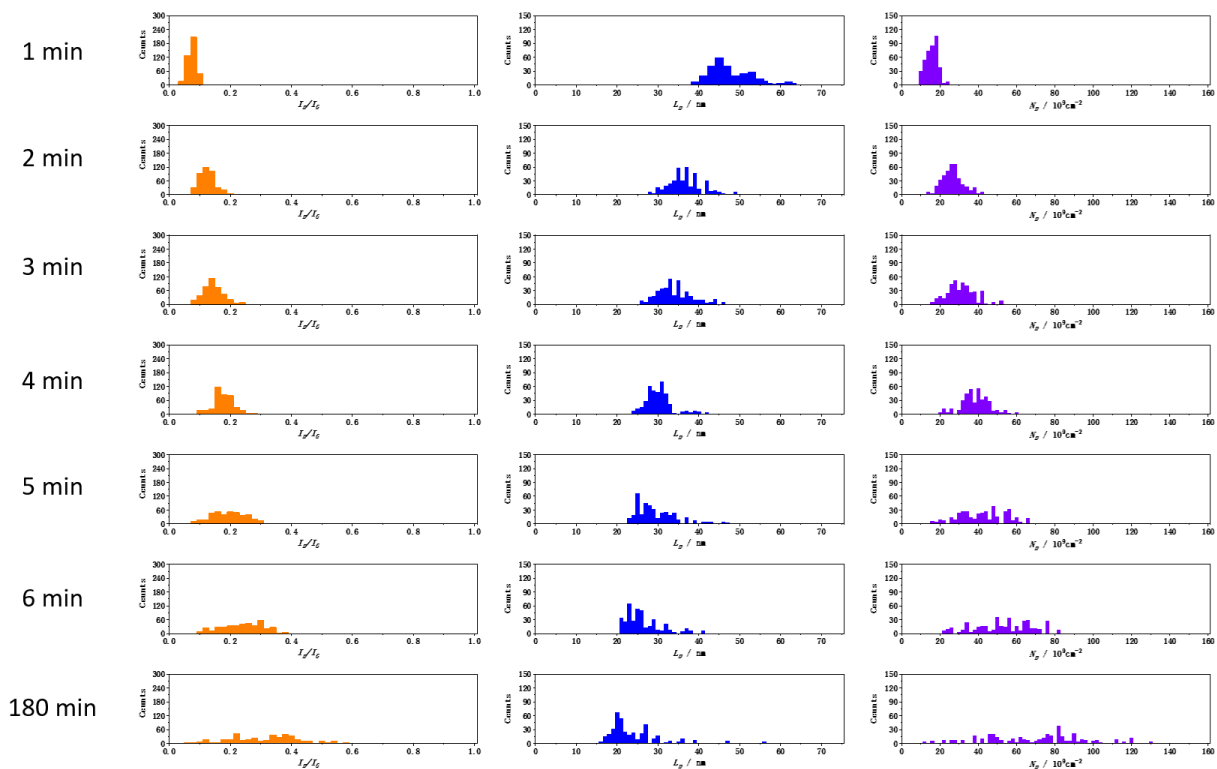


Figure S11. Histograms of (A) Raman I_D/I_G (B) L_D , and (C) n_D of G/SiO₂/Si after reacting with MAH at 50 °C for different lengths of time. Results were from ~400 data points on 2 sets of independent samples.

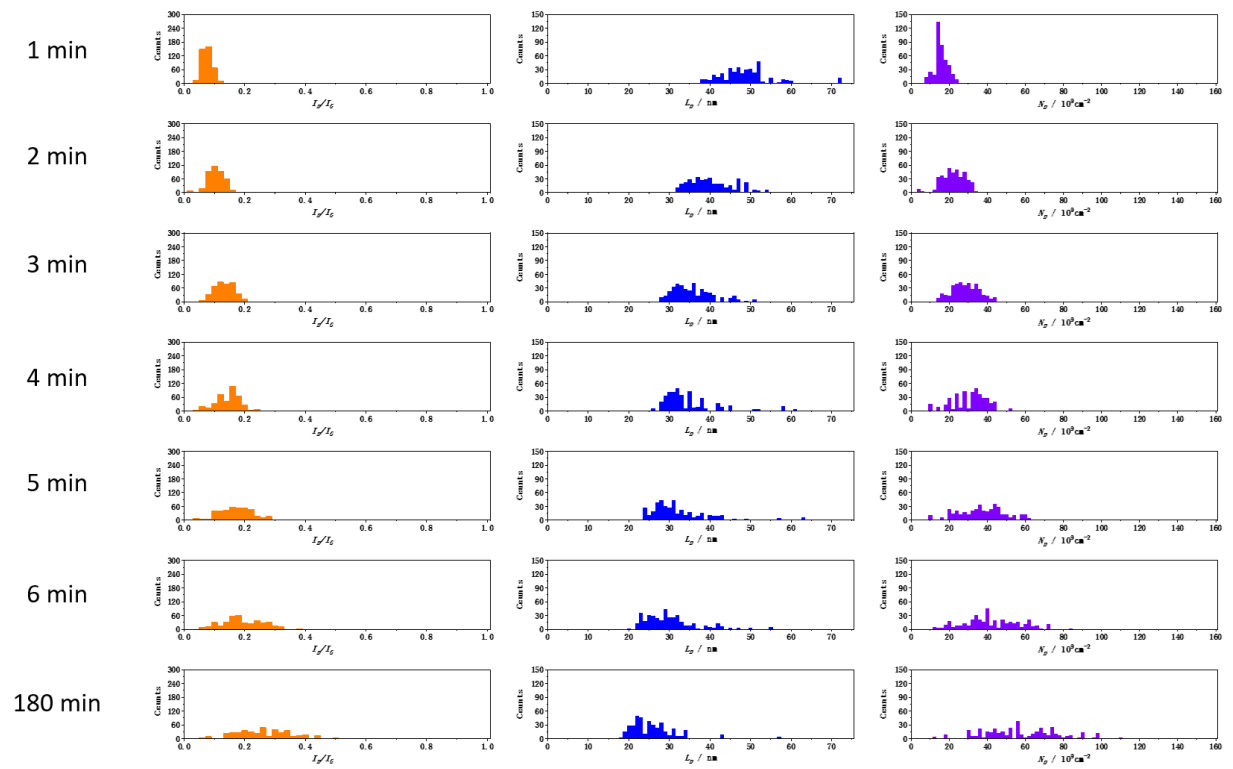


Figure S12. Histograms of (A) Raman I_D/I_G (B) L_D , and (C) n_D of G/Cu after reacting with MAH at 50 °C for different lengths of time. Results were from ~400 data points on 2 sets of independent samples.

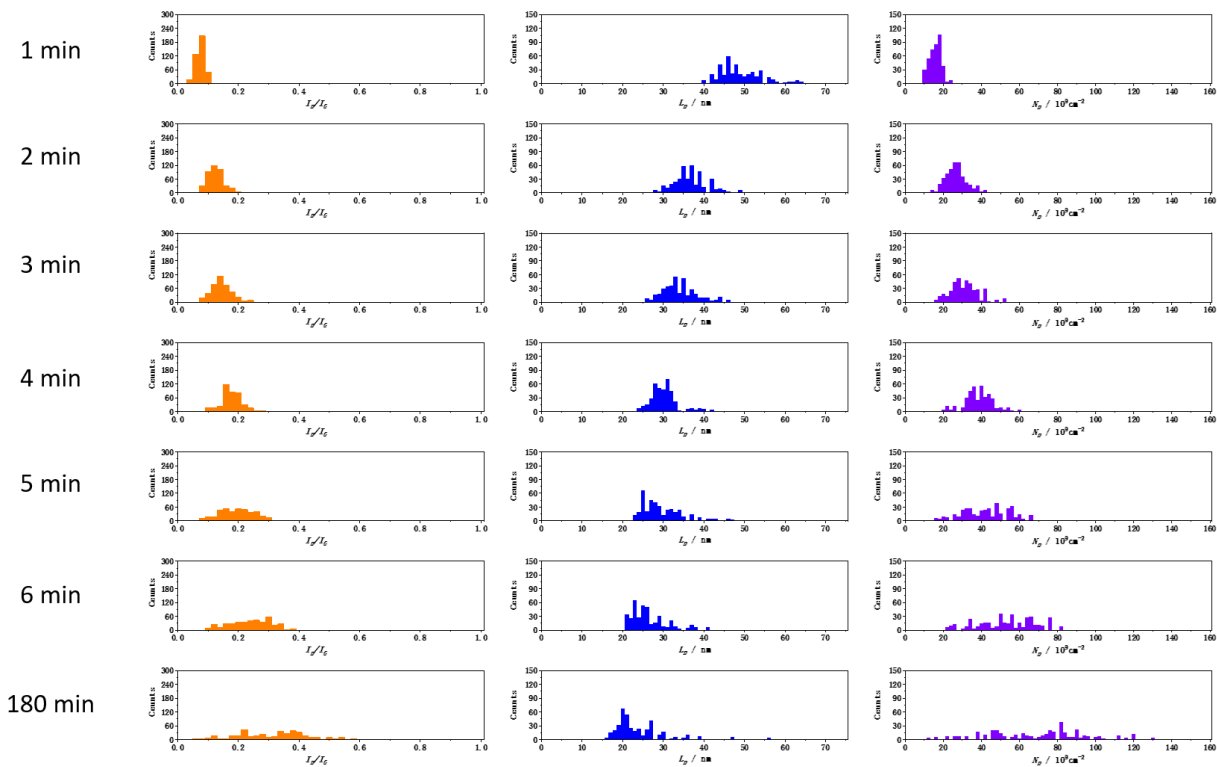


Figure S13. Histograms of (A) Raman I_D/I_G (B) L_D , and (C) n_D of G/Ni after reacting with MAH at 50 °C for different lengths of time. Results were from ~400 data points on 2 sets of independent samples.

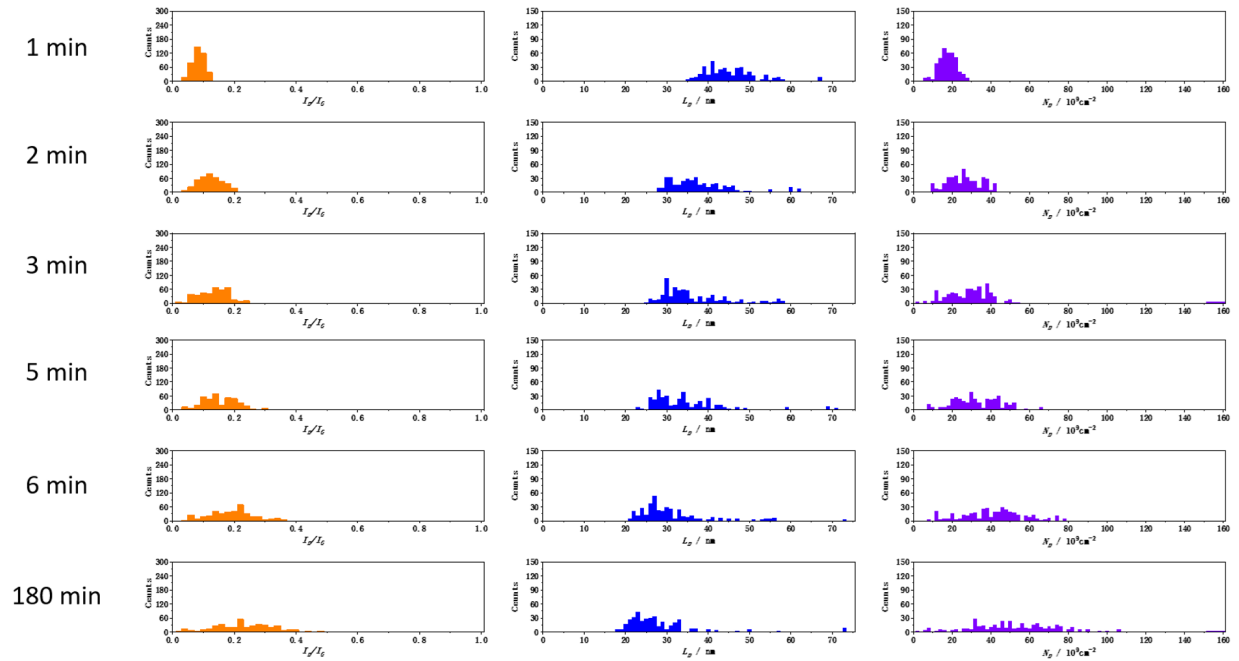


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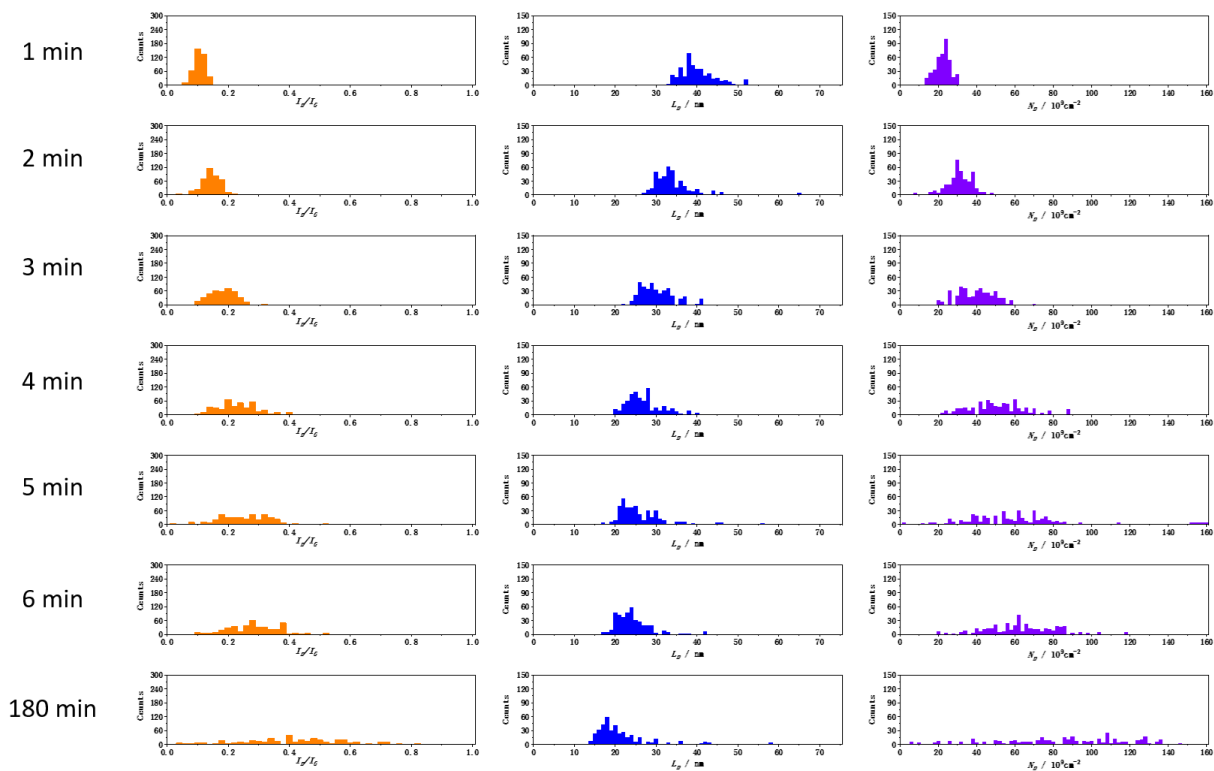


Figure S15. Histograms of (A) Raman I_D/I_G (B) L_D , and (C) n_D of G/Cu after reacting with MAH at 100 °C for different lengths of time. Results were from ~400 data points on 2 sets of independent samples.

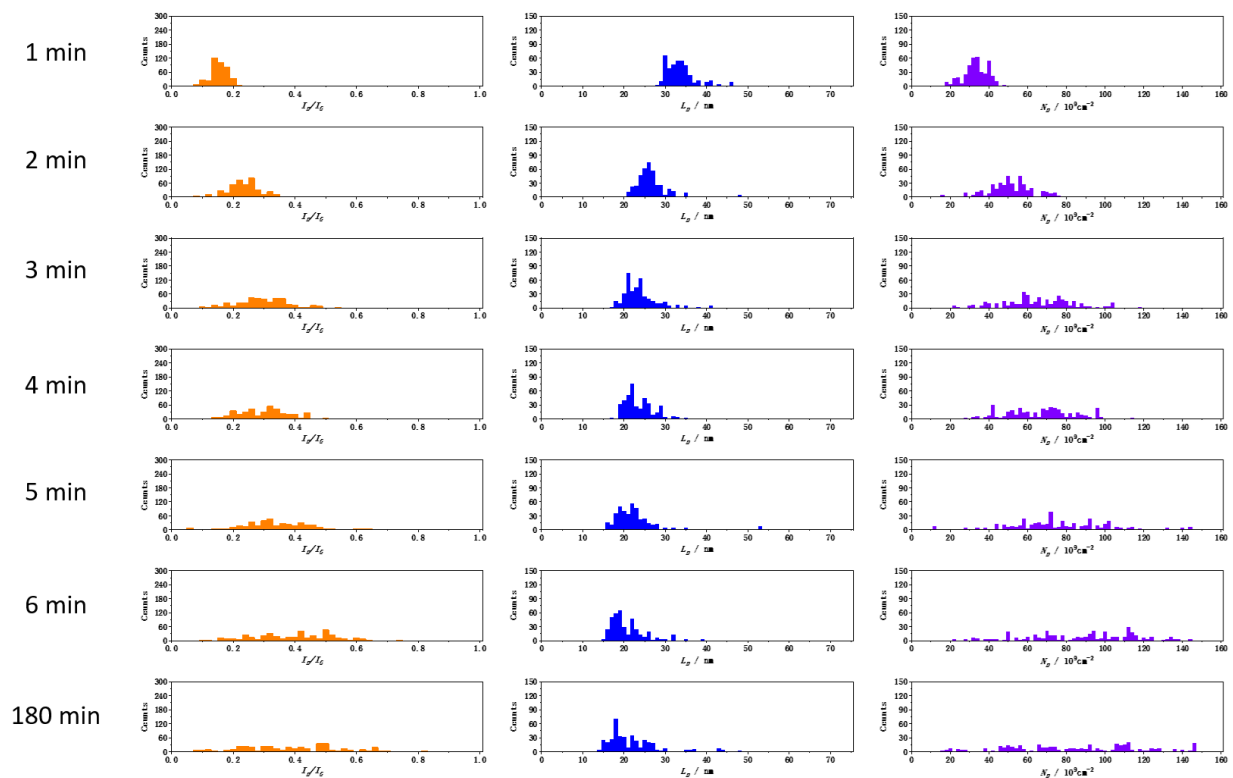


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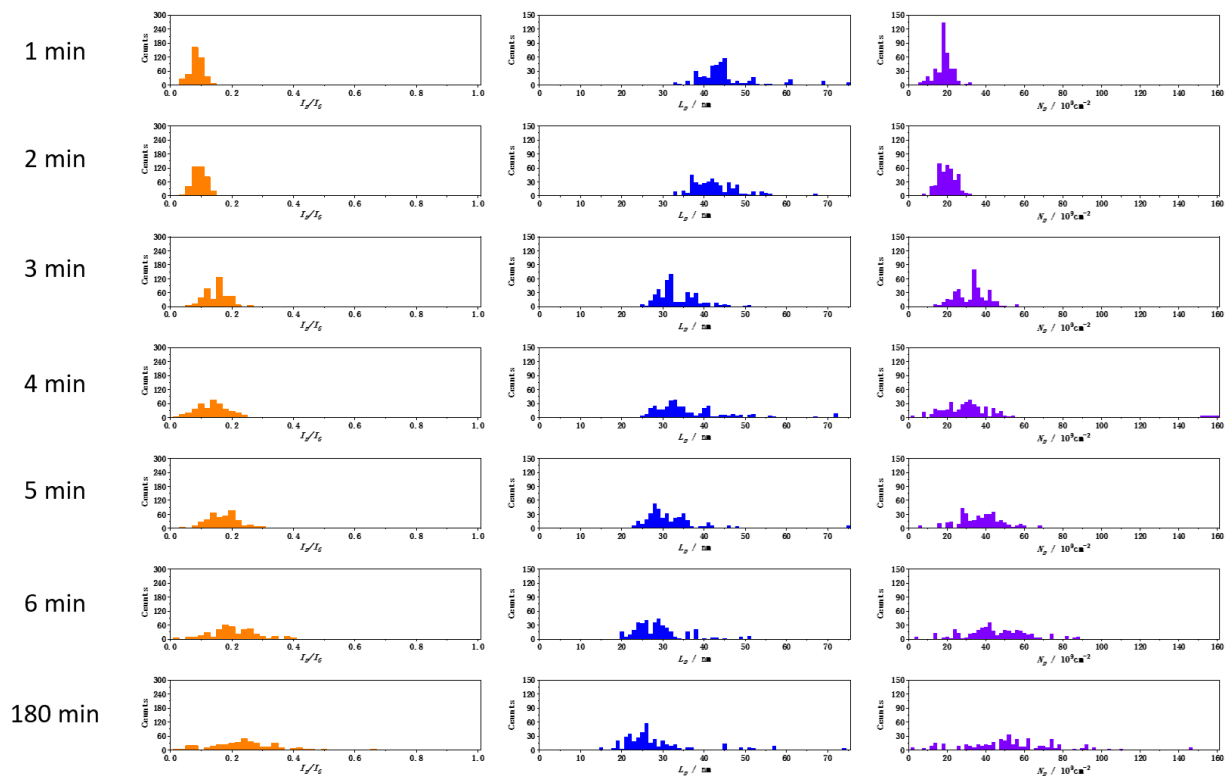


Figure S17. Histograms of (A) Raman I_D/I_G (B) L_D , and (C) n_D of G/SiO₂/Si after reacting with MAH at 150 °C for different lengths of time. Results were from ~400 data points on 2 sets of independent samples.

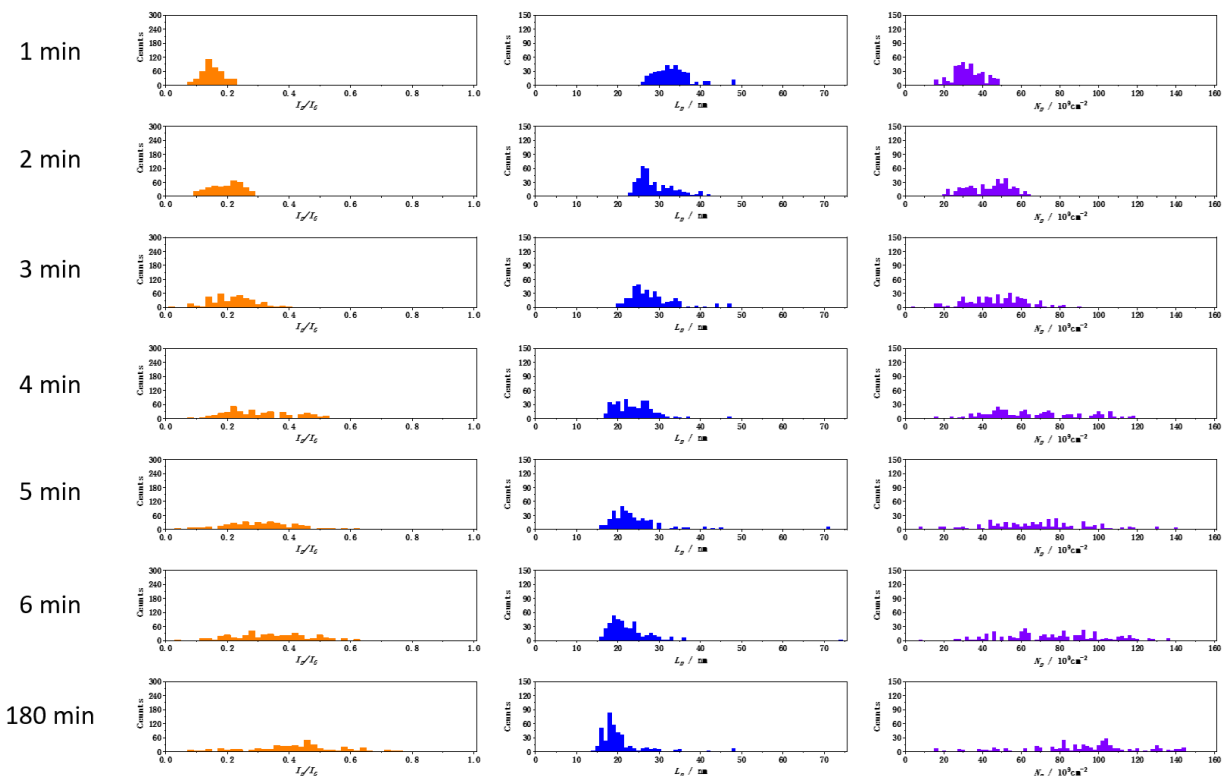


Figure S18. Histograms of (A) Raman I_D/I_G (B) L_D , and (C) n_D of G/Cu after reacting with MAH at 150 °C for different lengths of time. Results were from ~400 data points on 2 sets of independent samples.

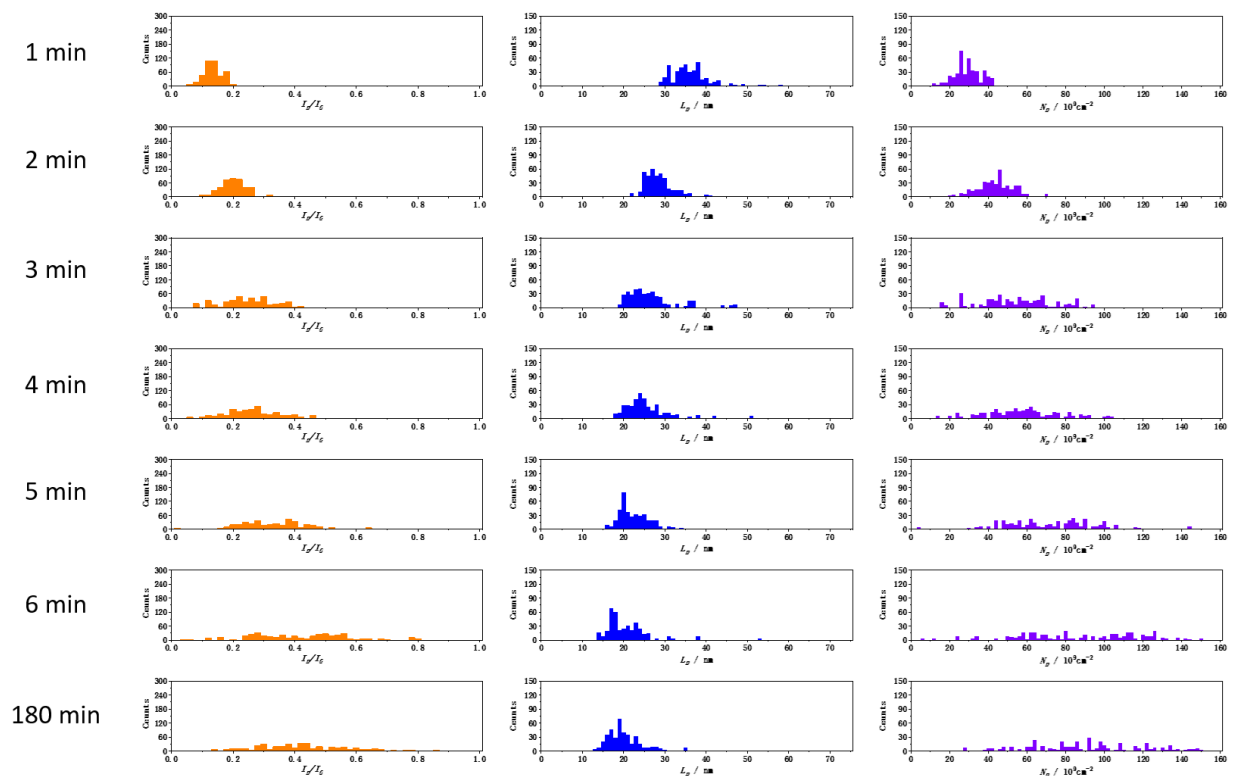


Figure S19. Histograms of (A) Raman I_D/I_G (B) L_D , and (C) n_D of G/Ni after reacting with MAH at 150 °C for different lengths of time. Results were from ~400 data points on 2 sets of independent samples.

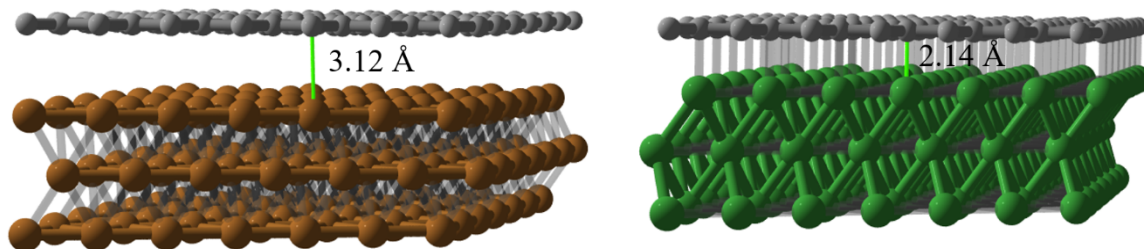


Figure S20. The interlayer distance of graphene adsorbed on Cu (111) (left) and Ni (111) (right) surface. The separation distances between the graphene layer and Cu(111)/Ni(111) are 3.12 Å and 2.14 Å, respectively.

Table S1. SCF energies (Ry) are given for the optimized geometries at gamma kpoints grid and single point energies of the gamma kpoints geometries at 3x3x1 kpoints. The total and absolute magnetizations are given where relevant.

	E (gamma)	E (3x3x1)
MAH	-149.1515856	-149.1516406
DMBD	-151.0272807	-151.0273226
IS-G	-1218.400886	-1218.351684
IS-G/Cu	-14101.59916	-14101.59214
IS-G/Ni	-13844.73961	-13844.73438
INT-G-MAH	-1367.588875	-1367.540684
INT-G-DMBD	-1369.464752	-1369.416331
INT-G/Cu-MAH	-14250.792	-14250.78504
INT-G/Cu-DMBD	-14252.66804	-14252.66227
INT-G/Ni-MAH	-13993.94873	-13993.94615
INT-G/Ni-DMBD	-13995.81891	-13995.81532
TS-G-MAH	N/A	N/A
TS-G-DMBD	N/A	N/A
TS-G/Cu-MAH	-14250.63611	-14250.63566
TS-G/Cu-DMBD	-14252.52043	-14252.51821
TS-G/Ni-MAH	-13993.86905	-13993.87298
TS-G/Ni-DMBD	-13995.72761	-13995.72874
FS-G-MAH	-1367.426527	-1367.38439
FS-G-DMBD	-1369.321521	-1369.279891
FS-G/Cu-MAH	-14250.63992	-14250.63934
FS-G/Cu-DMBD	-14252.53545	-14252.53339
FS-G/Ni-MAH	-13993.87884	-13993.88011
FS-G/Ni-DMBD	-13995.7625	-13995.76658

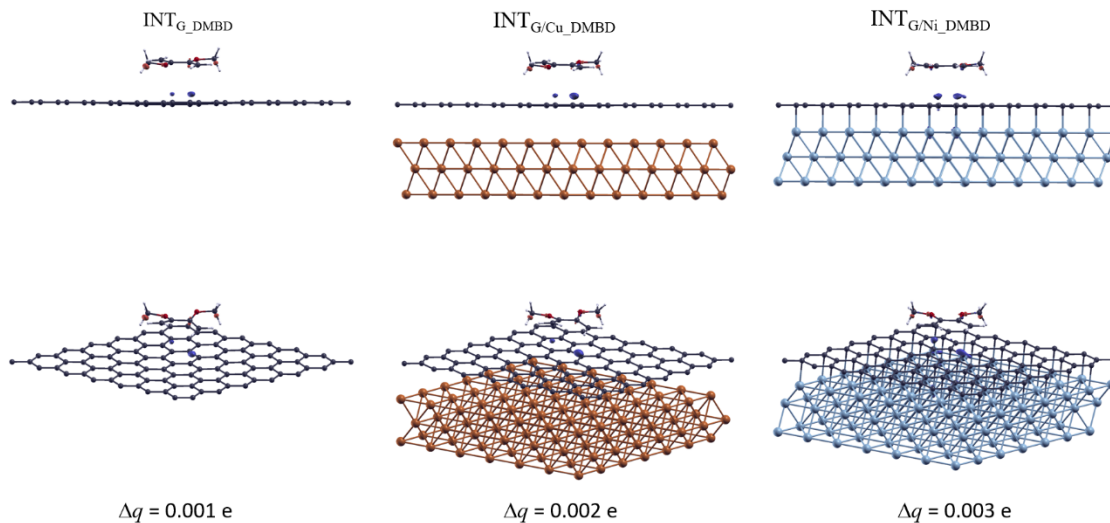


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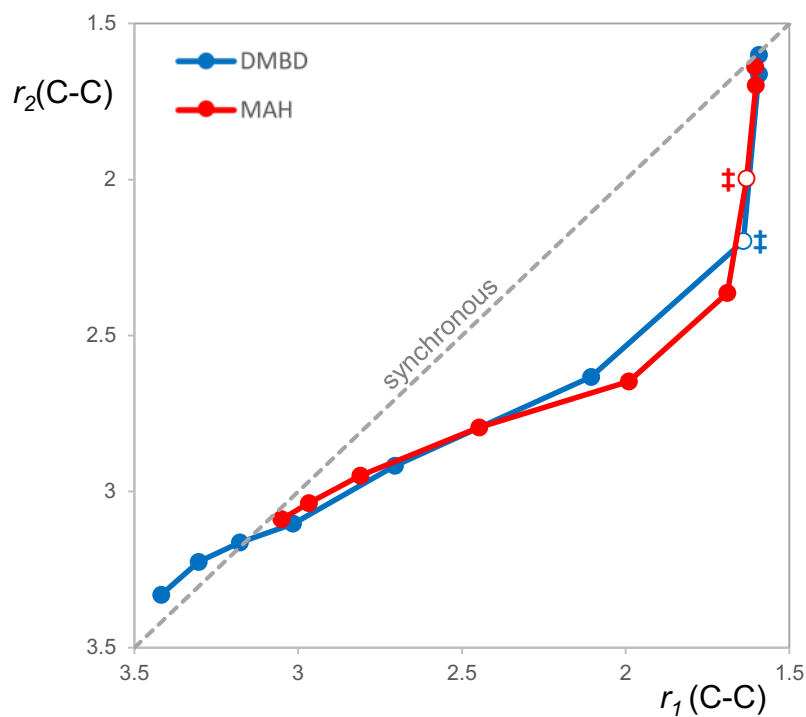


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Table S2. Geometry structure for all the optimized compounds and transition states

MAH				C	3.472344781	0.461030032	14.031275344
C	5.1533953379	6.7311102804	17.0580636875	C	2.240704349	1.172171699	14.018962074
C	5.4377930976	8.1867579228	16.9444160329	C	4.704167228	2.594482835	14.002054430
C	4.2722382127	8.8449187068	16.9507613462	C	3.472531534	3.305713589	13.984589861
C	3.1735182023	7.8491639486	17.0689074054	C	3.472473347	4.727969389	13.959266517
H	6.4517428760	8.5718451041	16.8702281747	C	2.240596262	5.439199438	13.962184615
H	4.0777299428	9.9123711696	16.8829544248	C	2.240558513	6.861737238	13.955265540
O	5.9112140849	5.7961820526	17.0958479327	C	1.008912948	7.572813326	13.984029971
O	1.9819458842	8.0151933922	17.1177858058	C	1.008847208	8.995245709	13.998245370
O	3.7573757737	6.5704964979	17.1226355100	C	-0.222663565	9.706284050	14.033794881
DMBD				C	-0.222583406	11.128625050	14.049541238
C	3.8275432159	8.4106297663	17.3693066100	C	-1.454548809	11.839900502	14.069161842
O	4.0753432021	9.7114318189	17.0317536412	C	-1.454575989	13.262321084	14.070143045
C	5.0633727525	7.5889666626	17.2971332979	C	-2.686382601	13.973609845	14.065165355
O	6.1544677634	8.2781435012	17.7459965935	C	5.935844534	0.461092480	14.048626789
C	5.0691803435	6.3262589327	16.8310120052	C	4.704169445	1.172294486	14.028807662
H	5.9677703139	5.7154079365	16.8111787037	C	7.167768992	2.594560206	14.026409679
H	4.1442015363	5.8976323972	16.4567194481	C	5.936120955	3.305779883	13.998656642
C	2.6290984552	7.9042496563	17.7166395446	C	5.936171524	4.728009068	13.971382610
H	1.7192076584	8.4993107074	17.7192351482	C	4.704462831	5.439132328	13.947882755
H	2.5612012441	6.8606131391	18.0097199579	C	4.704634703	6.861574704	13.931816324
C	2.9513747768	10.5890736307	17.0581677557	C	3.472275436	7.573090861	13.936367352
C	7.4134051690	7.6147956763	17.6326240980	C	3.472434327	8.995361956	13.945435369
H	3.3326589558	11.5860052827	16.8123755617	C	2.240876746	9.706469313	13.979495157
H	2.4892624710	10.5986347602	18.0588029110	C	2.240666909	11.128828794	14.002886586
H	2.1972327663	10.2767768898	16.3161706835	C	1.009147492	11.839849495	14.036107809
H	8.1642163433	8.3202636293	18.0049331977	C	1.009151986	13.262099730	14.048993590
H	7.6234598015	7.3591570900	16.5805798403	C	-0.222763694	13.973494490	14.062642620
H	7.4295884629	6.6925736461	18.2374464328	C	8.399498994	0.461033836	14.057802340
IS-G				C	7.167692162	1.172322091	14.046728395
C	2.240568617	2.594568590	14.000698504	C	9.631389396	2.594674906	14.052635883
C	1.008943960	3.305677995	14.002338540	C	8.399490936	3.306006324	14.033518178
C	1.008880577	4.728130112	13.988631831	C	8.399634833	4.728168119	14.017329188
C	-0.222849499	5.439168061	14.008153761	C	7.168103783	5.439180236	13.981863159
C	-0.222806139	6.861706411	14.008650539	C	7.168057048	6.861784943	13.964369611
C	-1.454546278	7.572698741	14.036015377	C	5.936359735	7.572887671	13.936447610
C	-1.454308213	8.995151699	14.046906239	C	5.936544596	8.995212904	13.936914104
C	-2.686317701	9.706311656	14.064149872	C	4.704107791	9.706760986	13.941156322
C	-2.686330244	11.128722685	14.071383143	C	4.704310894	11.129063441	13.965736105
C	-3.918213645	11.839913825	14.067408290	C	3.472659696	11.839977675	13.994029819
C	-3.918211936	13.262359463	14.062190818	C	3.472625140	13.262303831	14.019596656
C	-5.149929709	13.973542681	14.045454614	C	2.240814331	13.973535980	14.041312746

C 10.863163366 0.460975392 14.052408116
C 9.631244390 1.172261028 14.056322507
C 12.095029257 2.594658541 14.060992566
C 10.863166145 3.305912263 14.059550081
C 10.863240705 4.728190030 14.055800622
C 9.631340546 5.439497851 14.033950587
C 9.631437438 6.861811922 14.022574418
C 8.399958807 7.572850477 13.988655349
C 8.399831429 8.995385914 13.983975091
C 7.168225927 9.706588988 13.959368864
C 7.168063499 11.128953591 13.975191871
C 5.936180172 11.840116125 13.977642560
C 5.936161472 13.262433885 14.004767685
C 4.704480467 13.973631712 14.020894804
C 13.326744893 0.461018561 14.039667423
C 12.094914661 1.172231387 14.052387662
C 14.558665367 2.594778355 14.046904347
C 13.326864126 3.305887732 14.058929208
C 13.326956155 4.728279775 14.060796922
C 12.095036439 5.439464995 14.061342797
C 12.095077123 6.861820193 14.057075868
C 10.863068797 7.572966300 14.041106987
C 10.863359765 8.995403774 14.037228470
C 9.631507576 9.706517215 14.013257372
C 9.631596234 11.129027516 14.016768713
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C 8.399763331 13.262579916 14.014546009
C 7.168076723 13.973684434 14.016047641
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C -0.222952761 2.594581500 14.021572807
C -1.454646590 3.305642897 14.034187815
C -1.454567681 4.728046444 14.032181052
C -2.686329732 5.439140786 14.049409302
C -2.686280832 6.861563534 14.050527439
C -3.918209505 7.572668245 14.059324136
C -3.918123294 8.995084698 14.062047391
C -5.150085032 9.706239493 14.054377852
C -5.149997535 11.128652389 14.054762434
C -6.381836961 11.839812455 14.037801511
C -6.381699071 13.262244322 14.036509839
C -7.613423247 13.973390479 14.025900610
C 1.008721872 0.461019023 14.023975829
C -0.222879832 1.172084644 14.025378779

IS-G/Cu
Cu 1.020342336 3.316994543 10.967757419
Cu 2.263706581 2.597564856 8.862672619
Cu 1.022353907 1.878258214 6.750759000
Cu -0.223078000 5.471174833 10.968071443
Cu 1.019753011 4.751688782 8.861864160
Cu -0.220993025 4.032343424 6.750759000
Cu -1.466051223 7.625476067 10.969676361
Cu -0.223693963 6.905517597 8.862077884
Cu -1.464339957 6.186428635 6.750759000
Cu -2.708393616 9.779834801 10.971367073
Cu -1.466269916 9.059580250 8.863570706
Cu -2.707686890 8.340513845 6.750759000
Cu -3.952287989 11.933319152 10.972596367
Cu -2.708971785 11.213688768 8.864729887
Cu -3.951033822 10.494599055 6.750759000
Cu -5.196116467 14.087026837 10.972036649
Cu -3.951976474 13.367719798 8.864821054
Cu -5.194380755 12.648684265 6.750759000
Cu 2.263617423 1.162436745 10.969758151
Cu 3.507807535 0.443450013 8.863849455
Cu -6.437727687 14.802769475 6.750759000
Cu 3.507612821 3.317162260 10.965653416
Cu 4.751931280 2.597653799 8.861805549
Cu 3.509333670 1.878423274 6.750759000
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Cu 3.507942387 4.751349646 8.859882939
Cu 2.265986738 4.032508485 6.750759000
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Cu 1.022639805 6.186593695 6.750759000
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Cu 1.020505149 9.060481392 8.860369896
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Cu -1.464054060 10.494764115 6.750759000
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Cu -3.950747924 14.802934535 6.750759000
Cu 5.994714105 3.317637399 10.965146630

Cu 7.240128141	2.598323354	8.862740452	Cu 9.726193301	5.471940923	10.968217768
Cu 5.996313433	1.878588335	6.750759000	Cu 10.970742870	4.752589603	8.863593615
Cu 4.751099978	5.472457204	10.960933040	Cu 9.726926026	4.033003665	6.750759000
Cu 5.996597534	4.752297407	8.860471063	Cu 8.482657364	7.626794957	10.966049451
Cu 4.752966500	4.032673545	6.750759000	Cu 9.727704780	6.906384369	8.862635971
Cu 3.507621095	7.626521638	10.960567712	Cu 8.483579093	6.187088876	6.750759000
Cu 4.752488536	6.906311061	8.858493265	Cu 7.238836715	9.781429131	10.965266496
Cu 3.509619568	6.186758755	6.750759000	Cu 8.483868737	9.060812772	8.861950730
Cu 2.264218919	9.781091330	10.963157384	Cu 7.240232161	8.341174086	6.750759000
Cu 3.508665838	9.061108073	8.860926529	Cu 5.995126977	11.935597437	10.966790080
Cu 2.266272635	8.340843965	6.750759000	Cu 7.240219438	11.215974436	8.862008454
Cu 1.021916387	11.934122552	10.967770144	Cu 5.996885228	10.495259296	6.750759000
Cu 2.265038599	11.215757133	8.861523265	Cu 4.751983556	14.088798411	10.970102298
Cu 1.022925703	10.494929175	6.750759000	Cu 5.996055078	13.370485722	8.862548134
Cu -0.220962279	14.087030522	10.970414788	Cu 4.753538296	12.649344506	6.750759000
Cu 1.022162652	13.369597479	8.863264677	Cu 12.212416805	1.163362982	10.971310297
Cu -0.220421229	12.649014386	6.750759000	Cu 13.455996498	0.445883284	8.863606871
Cu 7.238777505	1.162638641	10.969298691	Cu 3.510191364	14.803429716	6.750759000
Cu 8.482920556	0.444411767	8.863973628	Cu 13.455759374	3.317430286	10.972112405
Cu -1.463768162	14.803099596	6.750759000	Cu 14.698996862	2.599207671	8.864559254
Cu 8.482385138	3.317418396	10.967463375	Cu 13.457252721	1.879083515	6.750759000
Cu 9.727232189	2.598703713	8.863498661	Cu 12.212602344	5.471949429	10.971551179
Cu 8.483293195	1.878753395	6.750759000	Cu 13.456044663	4.752949851	8.864727527
Cu 7.239001618	5.472278782	10.963842977	Cu 12.213905788	4.033168726	6.750759000
Cu 8.484478023	4.752418640	8.861937868	Cu 10.969342930	7.626577449	10.970682851
Cu 7.239946263	4.032838605	6.750759000	Cu 12.213496963	6.906618196	8.864546239
Cu 5.995238957	7.627048678	10.960667442	Cu 10.970558856	6.187253936	6.750759000
Cu 7.240779498	6.906377020	8.860196857	Cu 9.725486623	9.780858794	10.969696728
Cu 5.996599330	6.186923815	6.750759000	Cu 10.970474315	9.060544489	8.864175023
Cu 4.751809962	9.781754876	10.960577190	Cu 9.727211923	8.341339146	6.750759000
Cu 5.996979110	9.061249404	8.859440160	Cu 8.481804580	11.934832985	10.969830075
Cu 4.753252398	8.341009025	6.750759000	Cu 9.726930321	11.215112734	8.863987684
Cu 3.508560248	11.935542420	10.965795999	Cu 8.483864991	10.495424356	6.750759000
Cu 4.752829836	11.216416470	8.860622372	Cu 7.238130118	14.088264074	10.970718543
Cu 3.509905466	10.495094236	6.750759000	Cu 8.483205847	13.369712087	8.864090993
Cu 2.265682663	14.088210967	10.970080735	Cu 7.240518059	12.649509566	6.750759000
Cu 3.509039806	13.370666446	8.862520768	Cu 14.698620930	1.163301775	10.971862332
Cu 2.266558533	12.649179446	6.750759000	Cu 15.942651772	0.445289494	8.864248120
Cu 9.725935202	1.162672195	10.970131967	Cu 5.997171126	14.803594776	6.750759000
Cu 10.969725294	0.445520362	8.863724658	Cu -1.466441956	3.316293260	10.970824643
Cu 1.023211601	14.803264656	6.750759000	Cu -0.223410128	2.597698430	8.863763333
Cu 10.969210197	3.317218514	10.970936987	Cu 15.944232483	1.879248576	6.750759000
Cu 12.213147718	2.599445277	8.864217733	Cu -2.709664330	5.470829311	10.970755784
Cu 10.970272958	1.878918455	6.750759000	Cu -1.467043207	4.751596409	8.863704662

Cu	14.700885551	4.033333786	6.750759000	C	7.167313338	2.682913943	14.068362736
Cu	-3.952744464	7.625714894	10.971701546	C	5.923779996	3.400902891	14.060065604
Cu	-2.709945713	6.905596589	8.864299363	C	5.924035708	4.837041268	14.049236072
Cu	13.457538618	6.187418996	6.750759000	C	4.680398900	5.555300425	14.043415127
Cu	-5.196106193	9.779728641	10.972684342	C	4.680404514	6.991582402	14.038681870
Cu	-3.952333600	9.059587996	8.864838694	C	3.436769551	7.709765437	14.040460201
Cu	12.214191686	8.341504206	6.750759000	C	3.436794705	9.146181148	14.043893805
Cu	-6.440029345	11.933278074	10.972469950	C	2.193183264	9.864259898	14.052202124
Cu	-5.195446600	11.213489789	8.865332699	C	2.193451274	11.300410019	14.061737604
Cu	10.970844754	10.495589416	6.750759000	C	0.949911118	12.018176950	14.075129391
Cu	-7.683715926	14.086819225	10.971527979	C	0.950242439	13.454166895	14.082438941
Cu	-6.438734387	13.367941278	8.864796561	C	-0.293197989	14.171717590	14.087339171
Cu	9.727497821	12.649674627	6.750759000	C	8.410449184	0.529164330	14.083775062
Cu	-0.223491734	1.162042868	10.971200074	C	7.167051234	1.246793463	14.078750416
Cu	1.020597386	0.443594769	8.864380194	C	9.654316524	2.683283760	14.079986096
Cu	8.484150889	14.803759837	6.750759000	C	8.411077174	3.401185747	14.070578906
C	2.192643704	2.682637768	14.071172695	C	8.411257070	4.837301548	14.064342342
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C	0.949092311	4.836937806	14.063219894	C	7.167936588	6.991683340	14.047841850
C	-0.294494949	5.555132060	14.071611323	C	5.924345795	7.709914216	14.042322269
C	-0.294311148	6.991351901	14.067549782	C	5.924195770	9.146248081	14.048101459
C	-1.537784885	7.709332495	14.078952550	C	4.680714476	9.864271592	14.048917290
C	-1.537557363	9.145522090	14.080837547	C	4.680644395	11.300454996	14.058772257
C	-2.780802720	9.863368459	14.090227779	C	3.437190611	12.018511806	14.064627089
C	-2.780722202	11.299467987	14.090887523	C	3.437391283	13.454424413	14.076987017
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C	-4.023933290	13.453245221	14.091510769	C	10.897544530	0.529540150	14.087039136
C	-5.267318748	14.171145816	14.091067225	C	9.654239454	1.247201268	14.084311786
C	3.436138857	0.528543699	14.083791396	C	12.141034060	2.683475629	14.088879960
C	2.192605865	1.246542032	14.082478933	C	10.897929881	3.401471170	14.084833952
C	4.679984375	2.682696296	14.064894610	C	10.897815452	4.837577176	14.082957371
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C	-1.537105094	12.017537811	14.088261510	C	4.680974253	14.172324933	14.083186457
C	-1.536900086	13.453614571	14.089258839	C	13.384406458	0.529587756	14.089049703
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C	13.384245827	4.837692840	14.088661406	Ni	-6.253792938	12.089223743	10.000000000
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C	12.141052276	6.992069725	14.087694321	Ni	-6.254323257	14.943430983	11.971863976
C	10.898035641	7.710283052	14.084079069	Ni	-7.489850394	14.230105151	10.000000000
C	10.897915992	9.146391603	14.087460509	Ni	3.633755875	0.670779358	13.959958814
C	9.654677145	9.864506192	14.080908252	Ni	3.634064961	2.097849815	11.971918241
C	9.654634035	11.300515687	14.086565984	Ni	2.398580438	1.384800067	10.000000000
C	8.411263292	12.018455931	14.081848506	Ni	2.397507791	2.811994950	13.959127316
C	8.411195560	13.454361411	14.088067696	Ni	2.398256328	4.238943424	11.971783934
C	7.167787232	14.172263386	14.087395340	Ni	1.162522982	3.525681474	10.000000000
C	15.871105930	0.529543822	14.090214285	Ni	1.161451276	4.952968905	13.958870770
C	14.627783739	1.247589785	14.090394169	Ni	1.162672591	6.380211690	11.972408107
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C	-7.754229547	14.171167986	14.092386301	Ni	-3.782120193	14.943575179	11.972613133
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Ni	1.161683197	0.670542344	13.960390530	Ni	4.870666534	1.384783429	10.000000000
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Ni	4.870126941	7.092869336	13.960697174	Ni	8.578752455	7.807377741	10.000000000
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Ni	3.633551491	9.233848085	13.960101529	Ni	7.342694999	9.948259148	10.000000000
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Ni	7.342118430	7.092430859	13.958777599	Ni	11.050838551	7.807361103	10.000000000
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Ni	6.105110988	9.233755617	13.959451968	Ni	9.814781095	9.948242511	10.000000000
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Ni	4.869404967	11.374728755	13.960271034	Ni	8.578723639	12.089123919	10.000000000
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Ni	3.634368688	14.943424310	11.972505727	C	1.159682739	0.670807177	16.097805715
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C	12.088132046	6.861177309	14.029545774	Cu	2.263045180	2.596696856	8.863950186
C	10.856467812	7.572256256	14.021045009	Cu	1.022040754	1.877670712	6.750759000
C	10.856129816	8.993842331	14.020032139	Cu	-0.223188092	5.469578183	10.971065075
C	9.624278726	9.704437257	14.002741825	Cu	1.019502065	4.750176626	8.863480811
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C	14.550689607	1.173377018	14.016628098	Cu	-1.466339796	9.057049271	8.864990584
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C	-1.454817966	3.306846844	14.017218854	Cu	-3.951854675	11.929772121	10.975504369
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C	3.816290596	8.399176006	17.244304079	Cu	3.507054727	4.750092855	8.861963405
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Cu	-0.220937587	8.338232273	6.750759000	Cu	4.751068878	11.212630366	8.862440299
Cu	-1.464885445	11.930266406	10.973753258	Cu	3.508692451	10.491886539	6.750759000
Cu	-0.222839722	11.211379744	8.863998718	Cu	2.264824555	14.083590835	10.972408492
Cu	-1.464054931	10.491726044	6.750759000	Cu	3.507771029	13.366238116	8.863609286
Cu	-2.708204545	14.083249595	10.974076092	Cu	2.265575107	12.645380311	6.750759000
Cu	-1.465002870	13.364674532	8.865214053	Cu	9.723618276	1.162078256	10.973358602
Cu	-2.707172275	12.645219815	6.750759000	Cu	10.966967824	0.444979118	8.865018516
Cu	4.750071127	1.162052552	10.971880341	Cu	1.022457763	14.798874082	6.750759000
Cu	5.994138476	0.443421569	8.864883267	Cu	10.966421525	3.315859660	10.973503874
Cu	-3.950289618	14.798713587	6.750759000	Cu	12.210171956	2.598192007	8.865545823
Cu	5.993548890	3.316072655	10.968761134	Cu	10.967535518	1.877991703	6.750759000
Cu	7.238305544	2.596995376	8.864205982	Cu	9.723407989	5.470272455	10.971308799
Cu	5.994788136	1.877831207	6.750759000	Cu	10.967640979	4.750961175	8.864952168
Cu	4.750176580	5.470491829	10.965005965	Cu	9.724418174	4.031485474	6.750759000
Cu	5.995025588	4.750285827	8.862455077	Cu	8.480167624	7.624754551	10.969047821
Cu	4.751670792	4.031324978	6.750759000	Cu	9.724899820	6.904213141	8.864035555
Cu	3.507055391	7.624691097	10.962968987	Cu	8.481300830	6.184979245	6.750759000
Cu	4.751231130	6.904162115	8.860902291	Cu	7.236793944	9.778357909	10.967400428
Cu	3.508553448	6.184818750	6.750759000	Cu	8.481845564	9.058018792	8.862750041
Cu	2.264100040	9.778421088	10.967878353	Cu	7.238183486	8.338473016	6.750759000
Cu	3.507239277	9.058620533	8.862110788	Cu	5.993287403	11.931637677	10.969160619
Cu	2.265436104	8.338312521	6.750759000	Cu	7.238008182	11.212249529	8.862879434
Cu	1.021327094	11.930932499	10.970802363	Cu	5.995066142	10.491966787	6.750759000
Cu	2.263747276	11.212354550	8.862694319	Cu	4.750200216	14.083877677	10.972340103
Cu	1.022318760	10.491806292	6.750759000	Cu	5.994207161	13.366258677	8.863734114
Cu	-0.221398049	14.083316418	10.973345019	Cu	4.751948798	12.645460558	6.750759000
Cu	1.021325273	13.365735056	8.864305167	Cu	12.209455419	1.162349852	10.973974126
Cu	-0.220798584	12.645300063	6.750759000	Cu	13.452853519	0.445162548	8.865097310
Cu	7.237162203	1.162101002	10.972573395	Cu	3.508831454	14.798954329	6.750759000
Cu	8.480816732	0.444121712	8.865207570	Cu	13.452342637	3.315863157	10.974685597
Cu	-1.463915928	14.798793834	6.750759000	Cu	14.695449319	2.597926746	8.865801666
Cu	8.480329324	3.316142313	10.971373806	Cu	13.453909208	1.878071950	6.750759000
Cu	9.724572389	2.597657899	8.864991345	Cu	12.209361935	5.470001345	10.974093158
Cu	8.481161827	1.877911455	6.750759000	Cu	13.452747719	4.751049133	8.865951668
Cu	7.237063335	5.470721325	10.967975437	Cu	12.210791865	4.031565721	6.750759000
Cu	8.481922461	4.750608664	8.863838780	Cu	10.966058694	7.624008964	10.973373649
Cu	7.238044483	4.031405226	6.750759000	Cu	12.210202185	6.904223682	8.865793936
Cu	5.994158821	7.625050248	10.964301715	Cu	10.967674521	6.185059492	6.750759000
Cu	7.238730462	6.904089271	8.861850681	Cu	9.722765835	9.777675033	10.972514078
Cu	5.994927139	6.184898997	6.750759000	Cu	10.967657162	9.057561552	8.865402743
Cu	4.750466732	9.778376116	10.966068698	Cu	9.724557177	8.338553264	6.750759000
Cu	5.994735724	9.058520995	8.861205745	Cu	8.479160259	11.930796486	10.972261839

Cu	9.724354329	11.211436167	8.865028817	C	3.435811869	3.401017640	14.060446417
Cu	8.481439833	10.492047035	6.750759000	C	3.435888551	4.836450221	14.044110315
Cu	7.235935289	14.083764103	10.973476612	C	2.193056900	5.554119363	14.047351649
Cu	8.480550413	13.365531471	8.865220181	C	2.192276722	6.988812730	14.036250743
Cu	7.238322489	12.645540806	6.750759000	C	0.950031475	7.706585180	14.052247107
Cu	14.694945845	1.162235200	10.974698232	C	0.949848832	9.141770757	14.057898476
Cu	15.938722106	0.444774808	8.865653232	C	-0.292885366	9.859739098	14.073477938
Cu	5.995205145	14.799034577	6.750759000	C	-0.293441539	11.295535236	14.079284919
Cu	-1.466487104	3.315373371	10.974020301	C	-1.536567500	12.013718777	14.087731800
Cu	-0.223554042	2.597005498	8.865299573	C	-1.536815069	13.449657111	14.088493682
Cu	15.940282899	1.878152198	6.750759000	C	-2.779940119	14.167798521	14.088982491
Cu	-2.709201333	5.469308992	10.974077323	C	5.921770419	0.529230472	14.082077631
Cu	-1.466710701	4.750298889	8.865141129	C	4.678724358	1.247420105	14.077580701
Cu	14.697165555	4.031645969	6.750759000	C	7.164575662	2.683034151	14.068781389
Cu	-3.952041747	7.623304721	10.975075197	C	5.921759559	3.401078951	14.058092291
Cu	-2.709418946	6.903581818	8.865804150	C	5.921602477	4.835955315	14.041811938
Cu	13.454048211	6.185139740	6.750759000	C	4.678849763	5.552919156	14.030252429
Cu	-5.195381628	9.776648869	10.975708432	C	4.678420991	6.988259413	14.020509466
Cu	-3.951789937	9.056852692	8.866368763	C	3.435592087	7.705927327	14.024789050
Cu	12.210930867	8.338633511	6.750759000	C	3.435795922	9.142272750	14.034662415
Cu	-6.438975816	11.929878556	10.975050465	C	2.192375901	9.859769507	14.051747013
Cu	-5.194470848	11.210253596	8.866415166	C	2.192531349	11.295496543	14.064296598
Cu	10.967813524	10.492127282	6.750759000	C	0.949463035	12.013750306	14.076358305
Cu	-7.682367563	14.082972421	10.974703486	C	0.949401310	13.449654176	14.082623318
Cu	-6.437741634	13.364195418	8.866103070	C	-0.293735931	14.167727507	14.086780055
Cu	9.724696180	12.645621053	6.750759000	C	8.407943121	0.529156981	14.083913876
Cu	-0.223685847	1.161830552	10.974515500	C	7.164879690	1.247283641	14.079262204
Cu	1.020176006	0.443492248	8.865743119	C	9.650931702	2.682824069	14.079694150
Cu	8.481578836	14.799114825	6.750759000	C	8.407764949	3.400652079	14.070601636
C	2.192715671	2.683080863	14.072116028	C	8.407419413	4.836180721	14.063724244
C	0.949614745	3.400849140	14.074561504	C	7.1644464518	5.553418535	14.048258652
C	0.949902187	4.836452801	14.064544167	C	7.165094428	6.988412144	14.044360688
C	-0.293096573	5.554016990	14.072080990	C	5.922086281	7.706614195	14.029962570
C	-0.292827886	6.989465742	14.067187537	C	5.922106188	9.143296430	14.033115614
C	-1.536125288	7.706831729	14.079178176	C	4.679621522	9.860604444	14.035597991
C	-1.536285922	9.142336479	14.080643138	C	4.679203956	11.296254904	14.055971667
C	-2.779564188	9.860127566	14.089737807	C	3.435652294	12.013953943	14.066758582
C	-2.779827872	11.295932769	14.090782648	C	3.435753721	13.449989135	14.078432331
C	-4.023010210	12.013911669	14.094013615	C	2.192516019	14.167804786	14.083573642
C	-4.023095789	13.449830301	14.091272152	C	10.894367038	0.529218384	14.086526587
C	-5.266240902	14.167902343	14.090617733	C	9.651153337	1.247058947	14.084186403
C	3.435632728	0.529346754	14.083358389	C	12.137714614	2.682848476	14.087851209
C	2.192494171	1.247317644	14.082346477	C	10.894364798	3.400472521	14.083671721
C	4.678783214	2.683258622	14.064388645	C	10.894377752	4.836177772	14.081663217

C	9.650897018	5.553666148	14.073735322	H	4.071577052	9.940975729	17.163232949
C	9.651444664	6.989208442	14.073956788	O	5.898503432	5.813133797	17.098061273
C	8.407944508	7.706650547	14.062590097	O	1.962748966	8.040055502	17.154842178
C	8.408435607	9.142617172	14.067688244	O	3.746077852	6.599787488	17.141352158
C	7.165143297	9.860774399	14.056541608	INT-G/Cu-DMBD			
C	7.165560126	11.296831303	14.068735232	Cu	1.0202793297	3.3118767343	10.9694660316
C	5.922392983	12.014599867	14.068312199	Cu	2.2637250677	2.5946290559	8.8616688323
C	5.922370545	13.450481899	14.080269104	Cu	1.0221950017	1.8776898973	6.7507590000
C	4.679054082	14.168044646	14.083308526	Cu	-0.2227974229	5.4653755415	10.9698472862
C	13.380955661	0.529419566	14.088460366	Cu	1.0200660290	4.7478966463	8.8611729876
C	12.137659536	1.247062324	14.088705188	Cu	-0.2209921951	4.0311415332	6.7507590000
C	14.624463007	2.683089686	14.089532438	Cu	-1.4652628963	7.6191780442	10.9709883904
C	13.381076205	3.400638625	14.089134728	Cu	-0.2227540792	6.9011558751	8.8616708376
C	13.381304881	4.836397345	14.088081618	Cu	-1.4641793920	6.1845931692	6.7507590000
C	12.137816865	5.553926897	14.086562598	Cu	-2.7080491926	9.7724890082	10.9717968887
C	12.138154704	6.989617086	14.087732990	Cu	-1.4654104585	9.0545660022	8.8625165236
C	10.894710913	7.707174187	14.084803544	Cu	-2.7073665888	8.3380448051	6.7507590000
C	10.895043362	9.142952035	14.088432779	Cu	-3.9516380025	11.9254506895	10.9714800808
C	9.651787934	9.860756410	14.083279266	Cu	-2.7081517238	11.2081866758	8.8631555734
C	9.651969995	11.296681253	14.087336052	Cu	-3.9505537856	10.4914964410	6.7507590000
C	8.408873599	12.014699629	14.082911457	Cu	-5.1953142242	14.0790064807	10.9703918658
C	8.408873768	13.450572996	14.088082868	Cu	-3.9513795107	13.3617131700	8.8628905814
C	7.165680480	14.168357254	14.087416919	Cu	-5.1937409825	12.6449480770	6.7507590000
C	15.867586034	0.529704304	14.090008130	Cu	2.2634851142	1.1583803467	10.9698661678
C	14.624284279	1.247302247	14.090225688	Cu	3.5075491762	0.4412131322	8.8623329449
C	-0.293559356	2.682834977	14.084439629	Cu	-6.4369281793	14.7983997129	6.7507590000
C	-1.536828743	3.400444900	14.086866606	Cu	3.5069054637	3.3117481410	10.9669966245
C	-1.536493608	4.836156269	14.082825036	Cu	4.7515241992	2.5947586751	8.8610567971
C	-2.779924088	5.553612561	14.086855719	Cu	3.5088227155	1.8778361707	6.7507590000
C	-2.779620971	6.989269879	14.086106057	Cu	2.2630587049	5.4653490681	10.9661069661
C	-4.023062997	7.706817582	14.090371214	Cu	3.5077011249	4.7481441562	8.8605298982
C	-4.022981510	9.142527111	14.092304197	Cu	2.2656355186	4.0312878066	6.7507590000
C	-5.266279444	9.860256113	14.094259270	Cu	1.0204547737	7.6191979899	10.9686453919
C	-5.266268407	11.296084288	14.094840327	Cu	2.2641395964	6.9016247379	8.8604840472
C	-6.509419844	12.014043175	14.093821600	Cu	1.0224483218	6.1847394426	6.7507590000
C	-6.509403695	13.449943088	14.092476691	Cu	-0.2220105229	9.7725541592	10.9704307849
C	-7.752524284	14.167931311	14.091563772	Cu	1.0210960220	9.0549330186	8.8612883080
C	0.949358040	0.529284687	14.088384156	Cu	-0.2207388751	8.3381910785	6.7507590000
C	-0.293812260	1.247081498	14.089128482	Cu	-1.4647506697	11.9255662927	10.9717856788
C	5.146762980	6.762103306	17.127097266	Cu	-0.2217688850	11.2085168283	8.8620225199
C	5.430080678	8.207252063	17.140596860	Cu	-1.4639260719	10.4916427145	6.7507590000
C	4.256994172	8.871165130	17.158846291	Cu	-2.7082225918	14.0789245106	10.9705126949
C	3.163608234	7.884778476	17.156022058	Cu	-1.4644933310	13.3619676308	8.8627994225
H	6.442984740	8.598322181	17.125311129	Cu	-2.7071132687	12.6450943504	6.7507590000

Cu	4.7505082696	1.1586066664	10.9692491105	Cu	1.0229549619	14.7988385332	6.7507590000
Cu	5.9948272350	0.4413504572	8.8621291391	Cu	10.9674387808	3.3125700258	10.9712720085
Cu	-3.9503004656	14.7985459864	6.7507590000	Cu	12.2114834789	2.5963981180	8.8630144385
Cu	5.9943850271	3.3120880443	10.9662238383	Cu	10.9687058567	1.8782749910	6.7507590000
Cu	7.2392102152	2.5950858525	8.8610385092	Cu	9.7249042014	5.4660294117	10.9685468686
Cu	5.9954504292	1.8779824441	6.7507590000	Cu	10.9694039349	4.7488616062	8.8621639570
Cu	4.7507275202	5.4656723500	10.9651762579	Cu	9.7255186599	4.0317266269	6.7507590000
Cu	5.9955662128	4.7486077901	8.8602296666	Cu	8.4818642042	7.6199904223	10.9656605813
Cu	4.7522632324	4.0314340801	6.7507590000	Cu	9.7265985592	6.9017576007	8.8609788978
Cu	3.5069619968	7.6195150306	10.9651736656	Cu	8.4823314630	6.1851782629	6.7507590000
Cu	4.7517353093	6.9019896433	8.8603940746	Cu	7.2383542706	9.7742310824	10.9659957694
Cu	3.5090760355	6.1848857160	6.7507590000	Cu	8.4827049288	9.0554918910	8.8606653057
Cu	2.2638908731	9.7734892984	10.9668378313	Cu	7.2391442662	8.3386298988	6.7507590000
Cu	3.5084339274	9.0557508136	8.8618923120	Cu	5.9947162996	11.9276587637	10.9680551448
Cu	2.2658888387	8.3383373520	6.7507590000	Cu	7.2388130574	11.2099461903	8.8610107643
Cu	1.0214723822	11.9261641586	10.9689304260	Cu	5.9959570694	10.4920815348	6.7507590000
Cu	2.2651460643	11.2093357668	8.8611502824	Cu	4.7512618160	14.0806271212	10.9700683885
Cu	1.0227016419	10.4917889879	6.7507590000	Cu	5.9949746895	13.3640585531	8.8619781759
Cu	-0.2213276000	14.0791072907	10.9701903634	Cu	4.7527698725	12.6455331707	6.7507590000
Cu	1.0223461122	13.3627829044	8.8620138106	Cu	12.2104679375	1.1593688857	10.9712815155
Cu	-0.2204855550	12.6452406239	6.7507590000	Cu	13.4541506627	0.4434819359	8.8626035667
Cu	7.2377113653	1.1586410329	10.9691568256	Cu	3.5095826757	14.7989848067	6.7507590000
Cu	8.4818686469	0.4417461388	8.8620637020	Cu	13.4538460825	3.3127232525	10.9715595097
Cu	-1.4636727518	14.7986922598	6.7507590000	Cu	14.6971647411	2.5963581866	8.8630927620
Cu	8.4812959059	3.3124862472	10.9686228765	Cu	13.4553335705	1.8784212644	6.7507590000
Cu	9.7258030121	2.5956013175	8.8620392378	Cu	12.2109490023	5.4663320174	10.9707909786
Cu	8.4820781430	1.8781287176	6.7507590000	Cu	13.4546953076	4.7492818082	8.8630529573
Cu	7.2386736183	5.4658063699	10.9643228464	Cu	12.2121463736	4.0318729004	6.7507590000
Cu	8.4833372205	4.7484698361	8.8604162486	Cu	10.9680774018	7.6198379798	10.9691504946
Cu	7.2388909461	4.0315803535	6.7507590000	Cu	12.2123846896	6.9021159921	8.8623654819
Cu	5.9951370974	7.6200626025	10.9637606759	Cu	10.9689591768	6.1853245363	6.7507590000
Cu	7.2395528695	6.9019074342	8.8595819438	Cu	9.7244708997	9.7733688271	10.9684166765
Cu	5.9957037493	6.1850319895	6.7507590000	Cu	10.9691455135	9.0553459314	8.8619519207
Cu	4.7516931712	9.7745400031	10.9660747363	Cu	9.7257719800	8.3387761723	6.7507590000
Cu	5.9956135351	9.0559132257	8.8603826190	Cu	8.4808703714	11.9269060299	10.9695852437
Cu	4.7525165524	8.3384836254	6.7507590000	Cu	9.7253201240	11.2092467352	8.8621316417
Cu	3.5080378995	11.9276184858	10.9672402271	Cu	8.4825847831	10.4922278082	6.7507590000
Cu	4.7519923888	11.2100295569	8.8608968415	Cu	7.2373823482	14.0803073781	10.9703020826
Cu	3.5093293556	10.4919352613	6.7507590000	Cu	8.4815199581	13.3633599026	8.8626654006
Cu	2.2649249976	14.0802664733	10.9698112624	Cu	7.2393975863	12.6456794442	6.7507590000
Cu	3.5086473437	13.3639604897	8.8615867339	Cu	14.6966791419	1.1594399278	10.9711750372
Cu	2.2661421588	12.6453868973	6.7507590000	Cu	15.9402882100	0.4430294284	8.8628517790
Cu	9.7241983582	1.1589365541	10.9701743493	Cu	5.9962103894	14.7991310801	6.7507590000
Cu	10.9682191451	0.4429162820	8.8622357340	Cu	-1.4660001460	3.3116807742	10.9708504997

Cu	-0.2231110692	2.5948186752	8.8625000534	C	-1.4925375703	13.3405186983	14.0851828261
Cu	15.9419612842	1.8785675379	6.7507590000	C	-2.7360345672	14.0585804616	14.0857823103
Cu	-2.7089463111	5.4654557555	10.9708066678	C	5.9661708103	0.4200936842	14.0829699027
Cu	-1.4661685581	4.7480303181	8.8624661806	C	4.7228126402	1.1378118794	14.0798663556
Cu	14.6987740874	4.0320191738	6.7507590000	C	7.2091207476	2.5743033775	14.0767112356
Cu	-3.9517317390	7.6192838601	10.9706342216	C	5.9657256349	3.2923252952	14.0649890803
Cu	-2.7085911751	6.9012685496	8.8626740152	C	5.9649921629	4.7281054769	14.0458409809
Cu	13.4555868905	6.1854708098	6.7507590000	C	4.7225444397	5.4458087020	14.0306990677
Cu	-5.1951762899	9.7724663228	10.9704640964	C	4.7227430594	6.8812931035	14.0198587055
Cu	-3.9513014840	9.0546629792	8.8628005222	C	3.4808373733	7.5982215516	14.0281658338
Cu	12.2123996937	8.3389224457	6.7507590000	C	3.4814913028	9.0334054821	14.0285422884
Cu	-6.4388464284	11.9254899440	10.9704446004	C	2.2385498502	9.7507808076	14.0408828663
Cu	-5.1946439687	11.2080761541	8.8628551368	C	2.2377082245	11.1870659989	14.0457490418
Cu	10.9692124969	10.4923740816	6.7507590000	C	0.9945745279	11.9048182557	14.0664664577
Cu	-7.6823151603	14.0789573721	10.9701022477	C	0.9941490201	13.3409130763	14.0758388240
Cu	-6.4381589265	13.3617977845	8.8628451418	C	-0.2494869984	14.0587981971	14.0843330905
Cu	9.7260253000	12.6458257176	6.7507590000	C	8.4528037709	0.4204594962	14.0860607877
Cu	-0.2230777079	1.1582058393	10.9704205858	C	7.2091492590	1.1383119388	14.0834465958
Cu	1.0204954464	0.4413941318	8.8627018770	C	9.6957177771	2.5742895555	14.0860387360
Cu	8.4828381032	14.7992773535	6.7507590000	C	8.4522145572	3.2922323134	14.0794788650
C	2.2364020628	2.5737277320	14.0778637813	C	8.4516483329	4.7282581866	14.0696754595
C	0.9930915706	3.2914855207	14.0804283538	C	7.2079579918	5.4462110110	14.0506145302
C	0.9932873579	4.7274581414	14.0722471816	C	7.2080573892	6.8818962839	14.0364287466
C	-0.2499566725	5.4447851811	14.0802788279	C	5.9651480995	7.5994862359	14.0250732172
C	-0.2490479466	6.8804156511	14.0775684148	C	5.9659381224	9.0342112669	14.0351718372
C	-1.4925387611	7.5979426362	14.0852634876	C	4.7236323376	9.7515884727	14.0327954126
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C	-2.7361892015	11.1871410575	14.0887805879	C	3.4803999729	13.3407713077	14.0679367223
C	-3.9798241859	11.9051409233	14.0891771878	C	2.2372498977	14.0588947638	14.0767201884
C	-3.9796821929	13.3406155603	14.0856279937	C	10.9392809304	0.4205520964	14.0846847081
C	-5.2231593791	14.0586198488	14.0862620538	C	9.6958412412	1.1385519865	14.0874378596
C	3.4793202020	0.4200512459	14.0838005010	C	12.1828350926	2.5740503363	14.0874266589
C	2.2359633610	1.1379669562	14.0857569392	C	10.9393663510	3.2919667319	14.0866858164
C	4.7229736857	2.5737378136	14.0694415302	C	10.9390576756	4.7278983987	14.0845227869
C	3.4798477491	3.2917623117	14.0653789759	C	9.6954255630	5.4457593229	14.0767097532
C	3.4803202446	4.7276764448	14.0483995545	C	9.6955616772	6.8814907487	14.0703430949
C	2.2367614720	5.4454557154	14.0562572685	C	8.4522876382	7.5992841460	14.0513405514
C	2.2377510017	6.8806076473	14.0468110784	C	8.4524806489	9.0347265443	14.0591669320
C	0.9948462521	7.5974970193	14.0628900419	C	7.2091463724	9.7519034939	14.0535153300
C	0.9954121235	9.0330635819	14.0606232496	C	7.2095894753	11.1871092333	14.0660977893
C	-0.2483342784	9.7509543305	14.0755008403	C	5.9663085212	11.9047913067	14.0641462976
C	-0.2488771972	11.1868512455	14.0762904252	C	5.9668937043	13.3404745329	14.0754353282
C	-1.4924612898	11.9049169668	14.0854053145	C	4.7239961562	14.0586879708	14.0767824470

C	13.4260453917	0.4202935394	14.0855688129	H	2.1764956852	10.4347499637	16.6417784373
C	12.1829589269	1.1383563225	14.0867930197	H	8.1953409193	8.4579010986	17.7223099804
C	14.6694868422	2.5741614606	14.0896476860	H	7.6026774541	7.1493323235	16.6375494911
C	13.4262053331	3.2919198863	14.0880530923	H	7.4653376770	6.9647260020	18.4184073865
C	13.4260131496	4.7279256140	14.0889127519	INT-G/Ni-MAH			
C	12.1825159825	5.4456930464	14.0878406862	Ni	1.161046704	0.670701128	13.962380386
C	12.1829140518	6.8812957567	14.0879340445	Ni	1.161686117	2.097994176	11.973661347
C	10.9394155038	7.5993188038	14.0816144561	Ni	-0.073518339	1.384372011	10.000000000
C	10.9396918026	9.0347455901	14.0820658471	Ni	-0.074529217	2.810930981	13.962465720
C	9.6962605820	9.7524526582	14.0758108478	Ni	-0.073971910	4.238348528	11.974044215
C	9.6961679389	11.1880246365	14.0823461010	Ni	-1.309239718	3.524595095	10.000000000
C	8.4527038961	11.9054765451	14.0798480314	Ni	-1.310763860	4.951231136	13.963468940
C	8.4532617775	13.3410797828	14.0864478016	Ni	-1.309608691	6.378359903	11.974266734
C	7.2100448327	14.0589065771	14.0856350066	Ni	-2.544961098	5.664818179	10.000000000
C	15.9124875916	0.4204322941	14.0901361368	Ni	-2.546821756	7.091628346	13.962718968
C	14.6694135393	1.1383621424	14.0893918382	Ni	-2.545639370	8.518248836	11.973298232
C	-0.2502318769	2.5732530834	14.0881464632	Ni	-3.780682477	7.805041264	10.000000000
C	-1.4934180003	3.2909700061	14.0892446134	Ni	-3.782576711	9.231271584	13.961935764
C	-1.4936361243	4.7268299416	14.0866448913	Ni	-3.781438323	10.658496904	11.973743570
C	-2.7367338665	5.4445243421	14.0899189568	Ni	-5.016403856	9.945264348	10.000000000
C	-2.7363731076	6.8801220213	14.0890896515	Ni	-5.018010199	11.371400943	13.962511288
C	-3.9798526950	7.5981113305	14.0904878203	Ni	-5.016921606	12.798596322	11.973336231
C	-3.9794754235	9.0336527727	14.0902346831	Ni	-6.252125235	12.085487433	10.000000000
C	-5.2231111130	9.7514973545	14.0886094696	Ni	-6.253535718	13.511840192	13.962098203
C	-5.2231894380	11.1872708508	14.0884529043	Ni	-6.252658844	14.939058529	11.973374747
C	-6.4667946378	11.9049227866	14.0881164250	Ni	-7.487846614	14.225710517	10.000000000
C	-6.4665225249	13.3404946965	14.0876953730	Ni	3.632403652	0.670039957	13.962342176
C	-7.7098708484	14.0582425005	14.0902473082	Ni	3.633003542	2.097778115	11.973704093
C	0.9927094885	0.4197235974	14.0899136139	Ni	2.397784382	1.384291159	10.000000000
C	-0.2505227028	1.1375762788	14.0911858808	Ni	2.396753525	2.809901422	13.962557892
C	3.8228549930	8.4291048180	17.3720025834	Ni	2.397458257	4.237792420	11.973520995
O	4.0866965379	9.7555303013	17.1784212723	Ni	1.162063003	3.524514243	10.000000000
C	5.0672354846	7.6099132372	17.3627645114	Ni	1.160102456	4.950625985	13.961352523
O	6.1802425864	8.3759264151	17.5620289932	Ni	1.160609016	6.377920983	11.971311709
C	5.0741609206	6.2775710798	17.1679166182	Ni	-0.073658376	5.664737328	10.000000000
H	5.9856557645	5.6878965086	17.1906473430	Ni	-0.075825769	7.091889726	13.961978377
H	4.1437193346	5.7573944988	16.9628115820	Ni	-0.073997736	8.518360853	11.973136841
C	2.5932975031	7.9091645005	17.5521394444	Ni	-1.309379755	7.804960412	10.000000000
H	1.6939383845	8.5167617407	17.5141279942	Ni	-1.312614031	9.232028060	13.961163914
H	2.4767345281	6.8461210701	17.7393490521	Ni	-1.310135538	10.658591095	11.973245885
C	2.9901736910	10.6543781686	17.3506421153	Ni	-2.545101134	9.945183497	10.000000000
C	7.4307404187	7.6859527566	17.5848202255	Ni	-2.546956789	11.372126173	13.961888679
H	3.3887330815	11.6543938581	17.1490617236	Ni	-2.545540955	12.798934547	11.973377475
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Ni	-3.781940082	13.511873140	13.962154119	Ni	-0.073938450	14.225467962	10.000000000
Ni	-3.781265370	14.939196208	11.973871292	Ni	11.046254584	0.671025993	13.961844436
Ni	-5.016543893	14.225629665	10.000000000	Ni	11.046459594	2.097620426	11.973338333
Ni	6.104240643	0.669882749	13.962203601	Ni	9.811692547	1.384048604	10.000000000
Ni	6.104540426	2.097912270	11.973590916	Ni	9.810068414	2.811267398	13.962702392
Ni	4.869087104	1.384210307	10.000000000	Ni	9.810254774	4.238034595	11.974454386
Ni	4.868252905	2.809119604	13.961485190	Ni	8.575971168	3.524271688	10.000000000
Ni	4.868725182	4.237786467	11.972414904	Ni	8.574706826	4.952288617	13.965049780
Ni	3.633365725	3.524433392	10.000000000	Ni	8.574978992	6.377535258	11.974123194
Ni	3.631865657	4.950520845	13.958518496	Ni	7.340249789	5.664494772	10.000000000
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Ni	2.397644346	5.664656476	10.000000000	Ni	7.338636712	8.517789231	11.975545517
Ni	2.394281387	7.092256205	13.953825032	Ni	6.104528409	7.804717857	10.000000000
Ni	2.396513744	8.519393933	11.970923170	Ni	6.103317245	9.233549152	13.960380368
Ni	1.161922966	7.804879560	10.000000000	Ni	6.104268026	10.658851991	11.971205688
Ni	1.158070022	9.233081350	13.961803659	Ni	4.868807030	9.944940941	10.000000000
Ni	1.160798670	10.658197677	11.972931766	Ni	4.868623316	11.372275548	13.959732495
Ni	-0.073798413	9.945102645	10.000000000	Ni	4.868111370	12.798726632	11.974020449
Ni	-0.076482848	11.372618499	13.961722201	Ni	3.633085651	12.085164026	10.000000000
Ni	-0.074070696	12.798647746	11.973662113	Ni	3.631937623	13.512674490	13.962727758
Ni	-1.309519792	12.085325729	10.000000000	Ni	3.632533589	14.938765172	11.973325047
Ni	-1.310284876	13.512199554	13.962351743	Ni	2.397364272	14.225387110	10.000000000
Ni	-1.309929220	14.939016529	11.973494194	Ni	13.517578753	0.670831989	13.961670189
Ni	-2.545241171	14.225548814	10.000000000	Ni	13.518084311	2.097587061	11.973294549
Ni	8.575140267	0.670610573	13.962495734	Ni	12.282995268	1.383967752	10.000000000
Ni	8.575159194	2.098014085	11.974112088	Ni	12.281690014	2.811042683	13.961904588
Ni	7.340389825	1.384129455	10.000000000	Ni	12.282096290	4.237522781	11.973422012
Ni	7.338876515	2.810779370	13.963457966	Ni	11.047273889	3.524190836	10.000000000
Ni	7.339147801	4.238311984	11.975037035	Ni	11.046062180	4.950955401	13.962760279
Ni	6.104668446	3.524352540	10.000000000	Ni	11.046433756	6.377597345	11.973753718
Ni	6.102918420	4.952221948	13.962938220	Ni	9.811552510	5.664413921	10.000000000
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Ni	4.868947067	5.664575624	10.000000000	Ni	9.810315099	8.517536908	11.974446252
Ni	4.865252740	7.092576084	13.955019763	Ni	8.575831131	7.804637005	10.000000000
Ni	4.867551675	8.518360623	11.971773428	Ni	8.574353552	9.230822489	13.963788373
Ni	3.633225688	7.804798709	10.000000000	Ni	8.575378543	10.657645551	11.973549674
Ni	3.631108877	9.235217329	13.957372431	Ni	7.340109752	9.944860090	10.000000000
Ni	3.632198519	10.659004526	11.971248504	Ni	7.340006224	11.372265072	13.960422627
Ni	2.397504309	9.945021793	10.000000000	Ni	7.339143970	12.799020970	11.973302107
Ni	2.395627523	11.372691610	13.960516113	Ni	6.104388373	12.085083174	10.000000000
Ni	2.396966062	12.798970495	11.973738542	Ni	6.103009192	13.512236420	13.963064179
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Ni	1.161173902	13.512147343	13.962383586	Ni	4.868666993	14.225306258	10.000000000
Ni	1.161009172	14.939113185	11.973499238	Ni	15.988817414	0.670619699	13.961925635

Ni	15.989582526	2.097259732	11.973270840	C	-2.547795808	11.370255332	16.101589138
Ni	14.754297990	1.383886900	10.000000000	C	-3.783605087	12.083804154	16.101601028
Ni	14.753299008	2.810796605	13.962009381	C	-3.783736559	13.510874441	16.101809497
Ni	14.754030153	4.237669132	11.973672649	C	-5.019470396	14.224409714	16.102319556
Ni	13.518576611	3.524109985	10.000000000	C	6.101610814	0.669744899	16.103824654
Ni	13.517346630	4.950825008	13.962104749	C	4.866063667	1.383494038	16.105382679
Ni	13.517994475	6.377847473	11.973763391	C	4.865788149	2.810344812	16.099911631
Ni	12.282855232	5.664333069	10.000000000	C	3.630358967	3.523502454	16.100174324
Ni	12.281265253	7.090584885	13.962636790	C	3.629809311	4.949745218	16.081246374
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Ni	11.047133852	7.804556153	10.000000000	C	2.394185983	7.088934331	16.064722773
Ni	11.045379987	9.230241978	13.962965696	C	1.159046351	7.802658098	16.077743705
Ni	11.046257603	10.657836192	11.974057267	C	1.159006406	9.229243225	16.084927438
Ni	9.811412473	9.944779238	10.000000000	C	-0.076043860	9.942653456	16.098806982
Ni	9.809949612	11.370706476	13.962443810	C	-0.076349857	11.369649893	16.101377745
Ni	9.810666996	12.798301357	11.973579225	C	-1.312041748	12.083397223	16.102629506
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Ni	8.574104642	13.511836111	13.961816469	C	-2.548138078	14.224251058	16.103660660
Ni	8.575199729	14.938700196	11.973343160	C	8.572826948	0.669411413	16.101967831
Ni	7.339969715	14.225225407	10.000000000	C	7.337107855	1.383251184	16.104530552
C	1.159215875	0.669892753	16.101825573	C	7.336759487	2.809990790	16.101384801
C	-0.076434299	1.383264858	16.102619619	C	6.101231209	3.523671794	16.093921181
C	-0.076216928	2.810224351	16.103323457	C	6.101420707	4.949625685	16.080335440
C	-1.312019581	3.523596752	16.103950313	C	4.865485461	5.662150869	16.062495319
C	-1.311781920	4.950392927	16.104172553	C	4.865968568	7.089761578	16.071137079
C	-2.547614022	5.663568737	16.104609956	C	3.630026038	7.801772187	16.066928072
C	-2.547500343	7.090318413	16.103572531	C	3.629651683	9.229442889	16.073767665
C	-3.783507558	7.803539761	16.102733472	C	2.394222143	9.942677499	16.085839810
C	-3.783493324	9.230349951	16.101662251	C	2.394526124	11.369707573	16.101941124
C	-5.019580634	9.943539660	16.101685438	C	1.159015183	12.083148733	16.104853728
C	-5.019428137	11.370534335	16.100253684	C	1.158852168	13.510070683	16.103020149
C	-6.255429256	12.083878087	16.100659034	C	-0.076915081	14.223850344	16.102506345
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C	-7.490953757	14.224341548	16.101183956	C	9.808313641	1.382783276	16.101187649
C	3.630543158	0.669929466	16.103546416	C	9.807918260	2.809841069	16.101206226
C	2.394873566	1.383424794	16.104808861	C	8.572109172	3.523522782	16.103030713
C	2.394947787	2.810326593	16.104383007	C	8.571583572	4.950163271	16.103694009
C	1.159380873	3.523688626	16.105180385	C	7.335977978	5.663624777	16.099567742
C	1.159332642	4.950300872	16.099434582	C	7.335821389	7.089433984	16.109768452
C	-0.076037936	5.663693303	16.102025448	C	6.100733022	7.802388514	16.112926788
C	-0.076112525	7.089991436	16.094794361	C	6.101316094	9.229189978	16.091758160
C	-1.311653568	7.803320183	16.102864839	C	4.866525579	9.943032477	16.079818683
C	-1.311811666	9.229918490	16.101470339	C	4.865649537	11.370353112	16.099147722
C	-2.547545010	9.943330489	16.103334814	C	3.629797592	12.083182973	16.108436885

C	3.629933060	13.509952602	16.106478582	Ni	-0.073356389	4.238184302	11.974328255
C	2.394318450	14.223574079	16.104116033	Ni	-1.309056425	3.524736395	10.000000000
C	13.515583760	0.668945196	16.100489199	Ni	-1.309218338	4.951365902	13.963361323
C	12.279806332	1.382537103	16.100357844	Ni	-1.308471832	6.378496177	11.974878529
C	12.279701632	2.809594951	16.100195067	Ni	-2.544668376	5.665021641	10.000000000
C	11.043778094	3.523029531	16.101785299	Ni	-2.544739088	7.091056911	13.964166570
C	11.043421654	4.949854495	16.102478660	Ni	-2.544607732	8.518250652	11.974440296
C	9.807319421	5.663063491	16.106875156	Ni	-3.780280328	7.805306886	10.000000000
C	9.807185898	7.089746878	16.107482681	Ni	-3.780455557	9.230296854	13.964272609
C	8.571332355	7.802505270	16.115701496	Ni	-3.780486835	10.658151112	11.974047879
C	8.572075155	9.229358939	16.112065604	Ni	-5.015892280	9.945592132	10.000000000
C	7.336471134	9.942835863	16.106422247	Ni	-5.016406247	11.371007982	13.961948011
C	7.336618206	11.369822188	16.104018838	Ni	-5.016545423	12.798749602	11.972183574
C	6.101198026	12.083430229	16.105796119	Ni	-6.251504231	12.085877378	10.000000000
C	6.101231206	13.510261268	16.104694173	Ni	-6.252616910	13.512173405	13.961010280
C	4.865455855	14.223548021	16.104705937	Ni	-6.252412705	14.939534483	11.972925068
C	15.986951226	0.669095339	16.101418052	Ni	-7.487116183	14.226162624	10.000000000
C	14.751244683	1.382530142	16.101449851	Ni	3.632444913	0.670255540	13.961147338
C	14.751348995	2.809562059	16.101462798	Ni	3.632970595	2.098073056	11.973583762
C	13.515518794	3.522847799	16.102418676	Ni	2.397868748	1.384502850	10.000000000
C	13.515555279	4.949768310	16.102310796	Ni	2.396920500	2.810066889	13.962981583
C	12.279521473	5.662953692	16.102472615	Ni	2.397980699	4.238353525	11.974499417
C	12.279531357	7.089773891	16.100998033	Ni	1.162256796	3.524788095	10.000000000
C	11.043290165	7.802947587	16.103625315	Ni	1.161824501	4.950195115	13.962842340
C	11.043580615	9.229807516	16.103766396	Ni	1.162540898	6.378522737	11.973489754
C	9.807594524	9.942803443	16.109019284	Ni	-0.073355155	5.665073341	10.000000000
C	9.807886817	11.369757920	16.103204907	Ni	-0.073665362	7.091112823	13.963224722
C	8.572319437	12.083324764	16.104660413	Ni	-0.073337936	8.518431455	11.973914564
C	8.572397392	13.510194093	16.101795175	Ni	-1.308967107	7.805358587	10.000000000
C	7.336765295	14.223746045	16.103803019	Ni	-1.310226092	9.231115322	13.962943297
C	5.191399183	6.727081341	19.046528797	Ni	-1.309159516	10.658298130	11.973662474
C	5.466177085	8.166296547	19.075530333	Ni	-2.544579059	9.945643833	10.000000000
C	4.283570775	8.829762517	19.066069126	Ni	-2.545358183	11.371280078	13.961910453
C	3.198795655	7.847087003	19.031584114	Ni	-2.544501260	12.798695315	11.973068477
H	6.476224502	8.563729217	19.101921009	Ni	-3.780191010	12.085929078	10.000000000
H	4.096492793	9.899444778	19.078522056	Ni	-3.780776797	13.511808716	13.959724092
O	5.942339621	5.771648830	19.026651952	Ni	-3.780177326	14.939780549	11.973092704
O	1.991501617	7.990156195	19.004150202	Ni	-5.015802962	14.226214324	10.000000000
O	3.788386997	6.561265647	19.0232323290	Ni	6.105051437	0.670125147	13.963264981
INT-G/Ni-DMBD				Ni	6.104855177	2.097745387	11.974285903
Ni	1.160953576	0.670639766	13.962977186	Ni	4.869181969	1.384554550	10.000000000
Ni	1.161684135	2.097846826	11.974112826	Ni	4.868914454	2.808092156	13.961744393
Ni	-0.073444473	1.384451149	10.000000000	Ni	4.869194142	4.237592937	11.972509515
Ni	-0.074059700	2.811021875	13.963186695	Ni	3.633570017	3.524839796	10.000000000

Ni	3.634042597	4.948330834	13.961603295	Ni	7.340584507	5.665228443	10.000000000
Ni	3.634002455	6.378285586	11.971636216	Ni	7.340822537	7.092203468	13.957220779
Ni	2.397958065	5.665125042	10.000000000	Ni	7.339884342	8.519240659	11.971933497
Ni	2.396705058	7.090443218	13.957749049	Ni	6.104972555	7.805513688	10.000000000
Ni	2.398261496	8.518575112	11.970860563	Ni	6.105879171	9.233331050	13.960285043
Ni	1.162346114	7.805410287	10.000000000	Ni	6.105210513	10.658802143	11.973378509
Ni	1.159795788	9.232498765	13.959296503	Ni	4.869360604	9.945798934	10.000000000
Ni	1.162006554	10.658899294	11.972034797	Ni	4.870351032	11.372444497	13.961467824
Ni	-0.073265838	9.945695533	10.000000000	Ni	4.869458254	12.798450409	11.973948156
Ni	-0.075531366	11.372980547	13.960605233	Ni	3.633748652	12.086084180	10.000000000
Ni	-0.073406891	12.799879178	11.973361927	Ni	3.634027927	13.512101728	13.962332623
Ni	-1.308877790	12.085980779	10.000000000	Ni	3.633441113	14.939140296	11.974033467
Ni	-1.309236291	13.512642386	13.962441277	Ni	2.398136700	14.226369426	10.000000000
Ni	-1.308527864	14.940086894	11.974374707	Ni	13.518226567	0.670005357	13.961592417
Ni	-2.544489741	14.226266025	10.000000000	Ni	13.518603217	2.097461718	11.972637387
Ni	8.576144954	0.670801266	13.964799188	Ni	12.283121631	1.384709651	10.000000000
Ni	8.576075891	2.097860004	11.975107467	Ni	12.282342418	2.810800672	13.960632108
Ni	7.340495189	1.384606250	10.000000000	Ni	12.282502070	4.238450927	11.973258294
Ni	7.340703765	2.809627172	13.963840675	Ni	11.047509679	3.524994897	10.000000000
Ni	7.339683184	4.237970021	11.973569547	Ni	11.046726266	4.951213383	13.963472675
Ni	6.104883238	3.524891496	10.000000000	Ni	11.046867590	6.378573358	11.974581266
Ni	6.104425308	4.948844134	13.960047344	Ni	9.811897728	5.665280143	10.000000000
Ni	6.103723847	6.378970394	11.971786404	Ni	9.811740132	7.091663121	13.962172105
Ni	4.869271286	5.665176742	10.000000000	Ni	9.811651985	8.518749736	11.973931907
Ni	4.867919394	7.090779447	13.957032687	Ni	8.576285776	7.805565389	10.000000000
Ni	4.869044819	8.518878577	11.971514438	Ni	8.578362693	9.232587225	13.961938531
Ni	3.633659334	7.805461988	10.000000000	Ni	8.575845005	10.658854115	11.975155870
Ni	3.631657205	9.232307357	13.957312824	Ni	7.340673824	9.945850635	10.000000000
Ni	3.634235203	10.658332992	11.971845010	Ni	7.342378778	11.373178010	13.964639342
Ni	2.398047383	9.945747234	10.000000000	Ni	7.340123607	12.798514370	11.975528780
Ni	2.396523270	11.373029217	13.957640371	Ni	6.105061873	12.086135880	10.000000000
Ni	2.398193768	12.799040531	11.972926195	Ni	6.105283126	13.512336161	13.963785800
Ni	1.162435431	12.086032479	10.000000000	Ni	6.104687776	14.938984667	11.974056268
Ni	1.161745104	13.512980845	13.962386717	Ni	4.869449921	14.226421126	10.000000000
Ni	1.162372951	14.939560868	11.974412090	Ni	15.989441178	0.670602494	13.962887464
Ni	-0.073176521	14.226317725	10.000000000	Ni	15.990099721	2.097849634	11.973008164
Ni	11.047073455	0.670472675	13.963545408	Ni	14.754434852	1.384761352	10.000000000
Ni	11.046783627	2.097389728	11.973612732	Ni	14.754397157	2.811024412	13.960219228
Ni	9.811808410	1.384657951	10.000000000	Ni	14.754570699	4.238451045	11.972599878
Ni	9.811147146	2.810606955	13.963775547	Ni	13.518822900	3.525046598	10.000000000
Ni	9.811548252	4.238150046	11.974452699	Ni	13.518583830	4.951456403	13.961165927
Ni	8.576196459	3.524943197	10.000000000	Ni	13.518648520	6.378593700	11.973844127
Ni	8.575340858	4.950371836	13.961754508	Ni	12.283210948	5.665331843	10.000000000
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Ni	12.283091371	8.518344061	11.974269726	C	2.397646556	5.662546158	16.103124686
Ni	11.047598997	7.805617089	10.000000000	C	2.397626894	7.088700259	16.082538677
Ni	11.048587875	9.231781943	13.963447888	C	1.162669236	7.801649364	16.098375293
Ni	11.046865473	10.658886092	11.973976763	C	1.162450825	9.228215879	16.094243520
Ni	9.811987045	9.945902335	10.000000000	C	-0.073082981	9.942087809	16.108679507
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Ni	9.811153502	12.799302311	11.973834423	C	-1.308978603	12.082625515	16.103677188
Ni	8.576375093	12.086187581	10.000000000	C	-1.308960557	13.509681474	16.102392909
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Ni	8.575856512	14.939525297	11.973972954	C	8.575453590	0.668142571	16.111301173
Ni	7.340763142	14.226472827	10.000000000	C	7.340044359	1.381803260	16.112720175
C	1.161472813	0.668165968	16.105366679	C	7.339533266	2.808637805	16.112171053
C	-0.074113137	1.381607914	16.107809511	C	6.104054049	3.521945602	16.110235573
C	-0.073746190	2.808581061	16.106729631	C	6.103616780	4.948653762	16.093517447
C	-1.309346611	3.522000183	16.102893928	C	4.868580777	5.661902478	16.078569500
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C	-3.780760324	7.802404585	16.111242440	C	2.398278343	9.941479491	16.076097104
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C	-6.252554557	12.082575486	16.101682006	C	-0.073453274	14.223332090	16.110848181
C	-6.252411829	13.509654333	16.098019434	C	11.046659924	0.667969519	16.105176871
C	-7.488145336	14.223138309	16.105000374	C	9.811047690	1.381648506	16.110632841
C	3.632817394	0.668318562	16.099438199	C	9.810782026	2.808593330	16.107393409
C	2.397144420	1.381883377	16.105196009	C	8.575117785	3.522023404	16.112741628
C	2.397357117	2.808807958	16.108396079	C	8.575017313	4.948922848	16.105465717
C	1.161897154	3.522235364	16.111653274	C	7.339060322	5.662148699	16.094807404
C	1.162187281	4.949139835	16.110027709	C	7.338974545	7.089242885	16.079190117
C	-0.073387209	5.662349055	16.110800128	C	6.103455034	7.803177303	16.069776808
C	-0.073233950	7.089040716	16.109021302	C	6.104140017	9.229860836	16.083672034
C	-1.308903744	7.802269736	16.112840755	C	4.869249429	9.942652464	16.082365009
C	-1.308853449	9.229016991	16.109867053	C	4.869323731	11.368995302	16.098982007
C	-2.544731435	9.942266487	16.108416898	C	3.633924676	12.082480910	16.098089317
C	-2.544628065	11.369193883	16.101280942	C	3.633316654	13.509515873	16.105644778
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C	-3.780649240	13.509733627	16.093895600	C	13.518141411	0.667936564	16.099757207
C	-5.016533660	14.223314389	16.094672605	C	12.282342754	1.381519359	16.098916926
C	6.104318362	0.668325347	16.103231173	C	12.282358320	2.808759297	16.096050920
C	4.868631636	1.381845313	16.103696535	C	11.046500596	3.522293318	16.102289154
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C	3.633008647	3.522223959	16.109107910	C	9.810727705	5.662577005	16.106355027
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C	8.575450930	7.803245071	16.090877684	Cu	1.0206139004	4.7513872494	8.8553537117
C	8.574873560	9.229901587	16.104107347	Cu	-0.2210765900	4.0311644830	6.7507590000
C	7.339265404	9.942968216	16.105364267	Cu	-1.4626128922	7.6245695123	10.9696494742
C	7.339497993	11.369270043	16.112517365	Cu	-0.2187100817	6.9065146999	8.8619625717
C	6.104326041	12.082437154	16.113827330	Cu	-1.4641939340	6.1846582540	6.7507590000
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C	4.868930017	14.222845447	16.107120890	Cu	-1.4642632717	9.0579021486	8.8622066916
C	15.989538679	0.668115422	16.104274008	Cu	-2.7073112780	8.3381520250	6.7507590000
C	14.753776043	1.381588085	16.098901622	Cu	-3.9520828059	11.9289690023	10.9704662565
C	14.754026029	2.808860058	16.096381764	Cu	-2.7085097566	11.2099953167	8.8642597863
C	13.518256514	3.522296861	16.095140223	Cu	-3.9504286210	10.4916457970	6.7507590000
C	13.518321719	4.949449021	16.098068987	Cu	-5.1948157688	14.0827200657	10.9693648497
C	12.282415540	5.662799090	16.102992356	Cu	-3.9510865722	13.3639590772	8.8652945957
C	12.282585659	7.089613261	16.107895488	Cu	-5.1935459650	12.6451395680	6.7507590000
C	11.046857276	7.802889586	16.110595725	Cu	2.2623439348	1.1619962559	10.9629815453
C	11.046629080	9.229543845	16.109785927	Cu	3.5074437743	0.4436665848	8.8618942842
C	9.810922097	9.942911863	16.112732350	Cu	-6.4366633090	14.7986333390	6.7507590000
C	9.810795774	11.369517090	16.108373802	Cu	3.5075217759	3.3147502968	10.9552158218
C	8.575141977	12.082818076	16.112807131	Cu	4.7537615457	2.5965430067	8.8596829933
C	8.575512085	13.509755919	16.108120111	Cu	3.5084144450	1.8777509600	6.7507590000
C	7.339856772	14.223156549	16.110066526	Cu	2.2624482618	5.4660568235	10.9481571907
C	3.804416687	8.427040555	19.274814620	Cu	3.5106715691	4.7520027486	8.8561244451
O	4.092088619	9.762463672	19.238691475	Cu	2.2652971010	4.0312447310	6.7507590000
C	5.047597301	7.599478352	19.286102963	Cu	1.0224640743	7.6264740037	10.9697878238
O	6.168648110	8.380372935	19.303045207	Cu	2.2684021019	6.9085880898	8.8695001564
C	5.060448068	6.252194351	19.283514892	Cu	1.0221797570	6.1847385020	6.7507590000
H	5.985168745	5.683260606	19.301614178	Cu	-0.2219887695	9.7780147413	10.9718262916
H	4.130748696	5.692750688	19.263696429	Cu	1.0231007278	9.0616223666	8.8697504306
C	2.557644808	7.916742065	19.307301832	Cu	-0.2209375870	8.3382322730	6.7507590000
H	1.672804599	8.546502959	19.307025254	Cu	-1.4645715342	11.9298198409	10.9707394181
H	2.405118617	6.842366992	19.335400926	Cu	-0.2240028134	11.2121935953	8.8619962781
C	2.990781111	10.658110175	19.391366635	Cu	-1.4640549310	10.4917260440	6.7507590000
C	7.418737425	7.706874465	19.451708766	Cu	-2.7079304112	14.0839524523	10.9705585634
H	3.412398734	11.666492236	19.318004648	Cu	-1.4645108186	13.3650468098	8.8640258143
H	2.506829086	10.512968520	20.371842679	Cu	-2.7071722750	12.6452198150	6.7507590000
H	2.243955888	10.512265248	18.594791160	Cu	4.7507733789	1.1626834727	10.9657723994
H	8.184403188	8.490666083	19.446022016	Cu	5.9951888756	0.4427596186	8.8621154077
H	7.596689528	7.007474037	18.618960932	Cu	-3.9502896180	14.7987135870	6.7507590000
H	7.448125938	7.148933314	20.402512375	Cu	5.9985200707	3.3148069529	10.9665765277
TS-G/Cu-MAH				Cu	7.2403840672	2.5951553230	8.8616259040
Cu	1.0179885179	3.3144115204	10.9578934269	Cu	5.9947881360	1.8778312070	6.7507590000
Cu	2.2637290607	2.5978862011	8.8579272775	Cu	4.7555524729	5.4663705998	10.9597909361
Cu	1.0220407540	1.8776707120	6.7507590000	Cu	5.9972766535	4.7508289980	8.8611321124
Cu	-0.2234671308	5.4709454793	10.9604713364	Cu	4.7516707920	4.0313249780	6.7507590000

Cu 3.5131500471	7.6256649302	11.0123465083	Cu 8.4813008300	6.1849792450	6.7507590000
Cu 4.7482817186	6.9100309929	8.8762074177	Cu 7.2428194724	9.7745050143	10.9592381640
Cu 3.5085534480	6.1848187500	6.7507590000	Cu 8.4826690856	9.0550520009	8.8606759081
Cu 2.2655009028	9.7772796468	11.0195388639	Cu 7.2381834860	8.3384730160	6.7507590000
Cu 3.5061087576	9.0596361818	8.8944152162	Cu 5.9964926405	11.9355565013	10.9457735953
Cu 2.2654361040	8.3383125210	6.7507590000	Cu 7.2382213049	11.2077395828	8.8555844961
Cu 1.0205840762	11.9300295361	10.9721013441	Cu 5.9950661420	10.4919667870	6.7507590000
Cu 2.2617371958	11.2075543347	8.8686450506	Cu 4.7480147309	14.0831194816	10.9604764438
Cu 1.0223187600	10.4918062920	6.7507590000	Cu 5.9935381807	13.3653226239	8.8539537606
Cu -0.2207360142	14.0828423083	10.9713978557	Cu 4.7519487980	12.6454605580	6.7507590000
Cu 1.0215848014	13.3635607923	8.8619586599	Cu 12.2083543998	1.1616537848	10.9702014454
Cu -0.2207985840	12.6453000630	6.7507590000	Cu 13.4516251262	0.4446204736	8.8609098006
Cu 7.2392650099	1.1612201212	10.9702761702	Cu 3.5088314540	14.7989543290	6.7507590000
Cu 8.4820881364	0.4425454141	8.8629716168	Cu 13.4512253540	3.3162184893	10.9720179946
Cu -1.4639159280	14.7987938340	6.7507590000	Cu 14.6937172849	2.5993272074	8.8617716284
Cu 8.4813727504	3.3160095580	10.9722673938	Cu 13.4539092080	1.8780719500	6.7507590000
Cu 9.7240920752	2.5976327076	8.8643295826	Cu 12.2088469161	5.4706489651	10.9730129955
Cu 8.4811618270	1.8779114550	6.7507590000	Cu 13.4519529073	4.7519121340	8.8655216999
Cu 7.2386770750	5.4701827428	10.9812144979	Cu 12.2107918650	4.0315657210	6.7507590000
Cu 8.4795363105	4.7522805797	8.8661457799	Cu 10.9662785376	7.6224016781	10.9721594702
Cu 7.2380444830	4.0314052260	6.7507590000	Cu 12.2102262791	6.9038263096	8.8643095040
Cu 6.0032813219	7.6187563422	10.9939132558	Cu 10.9676745210	6.1850594920	6.7507590000
Cu 7.2351762873	6.9061367636	8.8688896377	Cu 9.7269181505	9.7735403692	10.9669313783
Cu 5.9949271390	6.1848989970	6.7507590000	Cu 10.9707651525	9.0559142484	8.8614063782
Cu 4.7508987410	9.7716945914	11.0275105217	Cu 9.7245571770	8.3385532640	6.7507590000
Cu 5.9870616851	9.0580198288	8.8785182625	Cu 8.4809128573	11.9302215828	10.9544261081
Cu 4.7518097950	8.3383927680	6.7507590000	Cu 9.7260830739	11.2086128592	8.8593244425
Cu 3.5053244365	11.9275520310	10.9685577512	Cu 8.4814398330	10.4920470350	6.7507590000
Cu 4.7497215693	11.2044842209	8.8715664927	Cu 7.2365817002	14.0870137808	10.9568348703
Cu 3.5086924510	10.4918865390	6.7507590000	Cu 8.4796966625	13.3647835966	8.8574245522
Cu 2.2651911754	14.0794582792	10.9703557787	Cu 7.2383224890	12.6455408060	6.7507590000
Cu 3.5078828946	13.3604248844	8.8609908972	Cu 14.6933975953	1.1630642633	10.9650434910
Cu 2.2655751070	12.6453803110	6.7507590000	Cu 15.9375164273	0.4464412137	8.8584549431
Cu 9.7245040506	1.1606020433	10.9708173485	Cu 5.9952051450	14.7990345770	6.7507590000
Cu 10.9672991161	0.4423639612	8.8637154423	Cu -1.4679706975	3.3164052998	10.9652780489
Cu 1.0224577630	14.7988740820	6.7507590000	Cu -0.2248840303	2.5980491131	8.8588866789
Cu 10.9649862534	3.3153268238	10.9731391454	Cu 15.9402828990	1.8781521980	6.7507590000
Cu 12.2087101921	2.5985197511	8.8655135254	Cu -2.7091305640	5.4699268600	10.9702031898
Cu 10.9675355180	1.8779917030	6.7507590000	Cu -1.4662775575	4.7519013122	8.8610972496
Cu 9.7225081652	5.4700538005	10.9746368709	Cu 14.6971655550	4.0316459690	6.7507590000
Cu 10.9647500640	4.7522611553	8.8656211540	Cu -3.9505382123	7.6224286889	10.9708579707
Cu 9.7244181740	4.0314854740	6.7507590000	Cu -2.7068314190	6.9041307259	8.8639789082
Cu 8.4808618296	7.6222112408	10.9820011160	Cu 13.4540482110	6.1851397400	6.7507590000
Cu 9.7223685336	6.9046372449	8.8661140602	Cu -5.1931452207	9.7746433232	10.9706815160

Cu	-3.9493467024	9.0560470933	8.8632022187	C	3.4371708491	7.6504596827	13.8966055354
Cu	12.2109308670	8.3386335110	6.7507590000	C	3.5014436734	9.0912196572	14.2944471683
Cu	-6.4386541779	11.9288262042	10.9655031872	C	2.2013407773	9.8373832522	14.1470668579
Cu	-5.1930361812	11.2095117491	8.8619302635	C	2.2027918972	11.2627069005	14.0932703513
Cu	10.9678135240	10.4921272820	6.7507590000	C	0.9581122456	11.9888327209	14.0748647787
Cu	-7.6824431849	14.0839122909	10.9628292917	C	0.9565417075	13.4269048106	14.0668098775
Cu	-6.4378982596	13.3637964689	8.8615705616	C	-0.2870264498	14.1457816186	14.0674590639
Cu	9.7246961800	12.6456210530	6.7507590000	C	8.4126840435	0.5084999374	14.0657742221
Cu	-0.2247245242	1.1631991995	10.9633925321	C	7.1694010314	1.2273132688	14.0613541666
Cu	1.0196933823	0.4441968616	8.8595209835	C	9.6515858222	2.6664198540	14.0677135073
Cu	8.4815788360	14.7991148250	6.7507590000	C	8.4075339963	3.3851041087	14.0633167721
C	2.1936718874	2.6583992289	14.0092807693	C	8.4046448924	4.8232623294	14.0738521833
C	0.9496141876	3.3766585987	14.0092711859	C	7.1599069447	5.5470432774	14.0864230460
C	0.9463318493	4.8100740318	13.9812483535	C	7.1601383989	6.9746362991	14.1436460460
C	-0.2926056948	5.5312544330	14.0134832537	C	5.8709279324	7.7231054376	14.2545974368
C	-0.2878454714	6.9700271581	14.0248565740	C	5.9280524428	9.1604091669	13.8668360315
C	-1.5339429006	7.6871332761	14.0520138417	C	4.7119620719	9.8623673807	13.8631212475
C	-1.5281382750	9.1220923413	14.0560214367	C	4.6886667689	11.2897815026	13.9154905047
C	-2.7724290849	9.8401622966	14.0629546534	C	3.4443807539	11.9984934117	14.0326738909
C	-2.7727934409	11.2759450696	14.0661080044	C	3.4409746378	13.4295106647	14.0405746914
C	-4.0167625017	11.9937289320	14.0625386889	C	2.1968156857	14.1497059185	14.0648336653
C	-4.0167263767	13.4290677958	14.0579152718	C	10.8974327670	0.5105268972	14.0667517860
C	-5.2602827870	14.1472991243	14.0502021444	C	9.6538204381	1.2293180404	14.0676690926
C	3.4402093071	0.5078749202	14.0410824252	C	12.1385296660	2.6655283268	14.0657783420
C	2.1958808509	1.2248738691	14.0349593271	C	10.8950066598	3.3841348591	14.0720012485
C	4.6807058223	2.6597349023	14.0152894725	C	10.8943097604	4.8192609333	14.0772838171
C	3.4365475258	3.3723377327	13.9834524487	C	9.6487936754	5.5381233122	14.0857347464
C	3.4332413838	4.8064967774	13.9238820225	C	9.6467296896	6.9724017498	14.0803757602
C	2.1897933889	5.5242112680	13.9214750196	C	8.3962648448	7.6881959029	14.0938811213
C	2.1875365935	6.9576383025	13.9202408085	C	8.4123775610	9.1298437879	14.0278110500
C	0.9510536803	7.6814115239	14.0128012792	C	7.1766938683	9.8534572087	13.9128476953
C	0.9680639339	9.1235545723	14.0800806682	C	7.1755858657	11.2883083218	13.9143203946
C	-0.2815826516	9.8391423306	14.0649307142	C	5.9316607002	12.0067979667	13.9149037456
C	-0.2846859756	11.2736520233	14.0768645029	C	5.9284832395	13.4401548080	13.9823232883
C	-1.5300771450	11.9931297585	14.0710604048	C	4.6839384793	14.1530151276	14.0208636869
C	-1.5303824958	13.4279852227	14.0674665799	C	13.3832680162	0.5130364536	14.0439698401
C	-2.7737929004	14.1472042818	14.0618715576	C	12.1397597886	1.2305895357	14.0620938155
C	5.9270060788	0.5074392339	14.0558850126	C	14.6251798999	2.6653867262	14.0512939005
C	4.6833869637	1.2254242967	14.0398918994	C	13.3815334573	3.3833307599	14.0609828417
C	7.1678878899	2.6624727908	14.0557227009	C	13.3819393542	4.8188838625	14.0640687300
C	5.9240936348	3.3827024940	14.0291950142	C	12.1373643586	5.5362329991	14.0721352268
C	5.9206567281	4.8121202770	14.0165502378	C	12.1374054108	6.9719712667	14.0698062272
C	4.6756206640	5.5208200536	13.9236239500	C	10.8930725237	7.6896533704	14.0702686815
C	4.6503566469	6.9498476220	13.9002818255	C	10.8989351870	9.1252806207	14.0639231583

C	9.6538884840	9.8428790031	14.0388223409	Cu	-2.7082743599	11.2083487937	8.8606313683
C	9.6584182875	11.2806307367	14.0186343636	Cu	-3.9505537859	10.4914964410	6.7507590000
C	8.4185773927	12.0023116786	13.9815556470	Cu	-5.1951497766	14.0791346462	10.9638328615
C	8.4154230141	13.4358652757	14.0085412169	Cu	-3.9509310092	13.3621129974	8.8603372100
C	7.1715392890	14.1542066778	14.0092992629	Cu	-5.1937409821	12.6449480770	6.7507590000
C	15.8710135693	0.5135687874	14.0349563100	Cu	2.2623715141	1.1582779760	10.9633708813
C	14.6264791778	1.2304101334	14.0433023130	Cu	3.5071305533	0.4409622314	8.8601227415
C	-0.2929598768	2.6618756184	14.0344579971	Cu	-6.4369281790	14.7983997130	6.7507590000
C	-1.5359691316	3.3811440054	14.0419598116	Cu	3.5063987036	3.3121893801	10.9675890873
C	-1.5361713798	4.8165313257	14.0390494929	Cu	4.7502827145	2.5944982135	8.8592556978
C	-2.7796618580	5.5346101340	14.0569145096	Cu	3.5088227159	1.8778361710	6.7507590000
C	-2.7772898106	6.9707706785	14.0596790968	Cu	2.2660032336	5.4702875972	10.9886494816
C	-4.0214969456	7.6881286286	14.0658989810	Cu	3.5110928262	4.7520859438	8.8763412900
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C	-5.2619884135	9.8412442680	14.0654227103	Cu	1.0238807833	7.6200329441	10.9781840426
C	-5.2598514099	11.2770235217	14.0588247913	Cu	2.2697350554	6.9040877268	8.8760070659
C	-6.5029597280	11.9953777230	14.0425081686	Cu	1.0224483220	6.1847394429	6.7507590000
C	-6.5034301810	13.4308335390	14.0414357382	Cu	-0.2221233336	9.7731766913	10.9638451843
C	-7.7464860992	14.1503252338	14.0349804269	Cu	1.0224449299	9.0544415234	8.8651036528
C	0.9530508926	0.5096336349	14.0404302021	Cu	-0.2207388750	8.3381910781	6.7507590000
C	-0.2909054454	1.2279225078	14.0410032165	Cu	-1.4639175199	11.9258855084	10.9629448245
C	5.0878874726	6.8787529502	16.7564853921	Cu	-0.2217594696	11.2087279688	8.8587171880
C	5.3535550000	8.1489581054	16.0362705676	Cu	-1.4639260720	10.4916427141	6.7507590000
C	4.0493145307	8.8856524624	15.9927112348	Cu	-2.7074095601	14.0783835109	10.9637078240
C	3.0791944110	8.0008638486	16.7197511021	Cu	-1.4637289961	13.3627338120	8.8592946258
H	6.2465219738	8.6762869515	16.3764115140	Cu	-2.7071132690	12.6450943501	6.7507590000
H	4.0425788417	9.9135742259	16.3663436425	Cu	4.7509703609	1.1582564711	10.9628237964
O	5.8493717834	6.0022781573	17.0843880036	Cu	5.9952676965	0.4418036824	8.8593557703
O	1.9318725507	8.2175387352	17.0194188990	Cu	-3.9503004659	14.7985459861	6.7507590000
O	3.6980283141	6.7747415753	17.0086536582	Cu	5.9917905124	3.3125516007	10.9636216356
TS-G/Cu-DMBD				Cu	7.2367271786	2.5979319645	8.8601655923
Cu	1.0228965499	3.3151617782	10.9710432218	Cu	5.9954504290	1.8779824440	6.7507590000
Cu	2.2647840982	2.5956353470	8.8605395294	Cu	4.7481293888	5.4709789611	11.0323972881
Cu	1.0221950020	1.8776898970	6.7507590000	Cu	5.9870870539	4.7538128477	8.8732205993
Cu	-0.2216854992	5.4660281156	10.9683679340	Cu	4.7522632321	4.0314340800	6.7507590000
Cu	1.0266542495	4.7519904935	8.8674926351	Cu	3.5054026459	7.6212359030	11.0356135194
Cu	-0.2209921950	4.0311415330	6.7507590000	Cu	4.7501962126	6.9027885636	8.8981683425
Cu	-1.4646030931	7.6195130150	10.9623299226	Cu	3.5090760351	6.1848857160	6.7507590000
Cu	-0.2181941482	6.9031087480	8.8639969953	Cu	2.2654540637	9.7707476130	10.9761413794
Cu	-1.4641793920	6.1845931690	6.7507590000	Cu	3.5091039527	9.0493561679	8.8752321073
Cu	-2.7078478955	9.7723657860	10.9634024686	Cu	2.2658888390	8.3383373520	6.7507590000
Cu	-1.4655855295	9.0548974851	8.8590850502	Cu	1.0223674603	11.9258837652	10.9607121671
Cu	-2.7073665890	8.3380448050	6.7507590000	Cu	2.2662337496	11.2049394768	8.8630073574
Cu	-3.9509016937	11.9256949474	10.9651585315	Cu	1.0227016420	10.4917889880	6.7507590000

Cu -0.2204096970	14.0794661209	10.9639293281	Cu 4.7527698721	12.6455331710	6.7507590000
Cu 1.0234641330	13.3621783422	8.8593358371	Cu 12.2109626192	1.1591905946	10.9651711354
Cu -0.2204855550	12.6452406240	6.7507590000	Cu 13.4542691104	0.4423791865	8.8608178200
Cu 7.2383539800	1.1584831831	10.9613522961	Cu 3.5095826760	14.7989848070	6.7507590000
Cu 8.4825375804	0.4427106018	8.8590928316	Cu 13.4541524331	3.3128382203	10.9654285315
Cu -1.4636727520	14.7986922600	6.7507590000	Cu 14.6982146434	2.5971026354	8.8612722667
Cu 8.4799776775	3.3136338302	10.9655150188	Cu 13.4553335709	1.8784212641	6.7507590000
Cu 9.7235716248	2.5979064415	8.8602058033	Cu 12.2107296262	5.4658987744	10.9634322561
Cu 8.4820781430	1.8781287179	6.7507590000	Cu 13.4549709058	4.7489229990	8.8603572305
Cu 7.2360183010	5.4673607890	10.9664067768	Cu 12.2121463739	4.0318729001	6.7507590000
Cu 8.4770978509	4.7522632588	8.8609015112	Cu 10.9683619902	7.6201510105	10.9609166593
Cu 7.2388909460	4.0315803531	6.7507590000	Cu 12.2120675069	6.9012362240	8.8592792080
Cu 5.9881203668	7.6193919205	11.0308806030	Cu 10.9689591770	6.1853245360	6.7507590000
Cu 7.2309381158	6.9070179948	8.8729136178	Cu 9.7248487226	9.7739932681	10.9622176195
Cu 5.9957037490	6.1850319891	6.7507590000	Cu 10.9690817667	9.0551791946	8.8590503340
Cu 4.7482705428	9.7699936479	10.9856028919	Cu 9.7257719800	8.3387761720	6.7507590000
Cu 5.9941190852	9.0508390499	8.8763530325	Cu 8.4802939051	11.9282418672	10.9631366576
Cu 4.7525165521	8.3384836251	6.7507590000	Cu 9.7257681270	11.2104026405	8.8598968115
Cu 3.5083667771	11.9262207544	10.9671032406	Cu 8.4825847830	10.4922278080	6.7507590000
Cu 4.7520685731	11.2029824416	8.8665852275	Cu 7.2366574483	14.0795198234	10.9653435716
Cu 3.5093293559	10.4919352610	6.7507590000	Cu 8.4812875195	13.3641216906	8.8597568183
Cu 2.2657591445	14.0800014690	10.9632036971	Cu 7.2393975860	12.6456794440	6.7507590000
Cu 3.5090310980	13.3603706444	8.8600809407	Cu 14.6968843308	1.1593597069	10.9667482981
Cu 2.2661421590	12.6453868970	6.7507590000	Cu 15.9400083811	0.4433294818	8.8611358210
Cu 9.7250876323	1.1596543788	10.9628280225	Cu 5.9962103891	14.7991310800	6.7507590000
Cu 10.9687533714	0.4430231746	8.8597271061	Cu -1.4654681411	3.3120647474	10.9646386407
Cu 1.0229549620	14.7988385330	6.7507590000	Cu -0.2204235363	2.5975179006	8.8621101806
Cu 10.9671755392	3.3131077100	10.9638715441	Cu 15.9419612840	1.8785675380	6.7507590000
Cu 12.2109054812	2.5968956579	8.8599099927	Cu -2.7087528037	5.4653975059	10.9644077264
Cu 10.9687058570	1.8782749910	6.7507590000	Cu -1.4628083122	4.7499833552	8.8609884156
Cu 9.7230650422	5.4670544161	10.9649236047	Cu 14.6987740871	4.0320191740	6.7507590000
Cu 10.9664305981	4.7499980503	8.8602531552	Cu -3.9515819059	7.6188752802	10.9645919328
Cu 9.7255186600	4.0317266270	6.7507590000	Cu -2.7073002814	6.9006946821	8.8601521116
Cu 8.4798143320	7.6223770774	10.9629906641	Cu 13.4555868909	6.1854708100	6.7507590000
Cu 9.7229380698	6.9029100810	8.8598646942	Cu -5.1941992194	9.7727569583	10.9639168936
Cu 8.4823314630	6.1851782630	6.7507590000	Cu -3.9515074777	9.0536616135	8.8596808207
Cu 7.2370315185	9.7743454433	10.9674978170	Cu 12.2123996940	8.3389224460	6.7507590000
Cu 8.4825983237	9.0573373965	8.8590065612	Cu -6.4385304094	11.9262649510	10.9639288175
Cu 7.2391442660	8.3386298990	6.7507590000	Cu -5.1944991411	11.2078093290	8.8602803023
Cu 5.9928447408	11.9232251684	10.9705590324	Cu 10.9692124970	10.4923740819	6.7507590000
Cu 7.2387206523	11.2087913287	8.8603814082	Cu -7.6823782364	14.0792520363	10.9665180450
Cu 5.9959570691	10.4920815350	6.7507590000	Cu -6.4384638304	13.3624313084	8.8599840367
Cu 4.7516916806	14.0796467064	10.9636643708	Cu 9.7260253000	12.6458257179	6.7507590000
Cu 5.9945138077	13.3605397876	8.8617047825	Cu -0.2231565467	1.1593573675	10.9654206224

Cu	1.0199292333	0.4419814073	8.8599971138	C	9.7004561037	2.5742432531	14.0395287795
Cu	8.4828381030	14.7992773531	6.7507590000	C	8.4573233376	3.2901170989	14.0257770634
C	2.2429893216	2.5718495629	14.0387015295	C	8.4533632999	4.7299789555	14.0265120599
C	0.9970266856	3.2908896497	14.0444274343	C	7.2165917050	5.4439852067	14.0447307799
C	0.9979765909	4.7273099354	14.0539488041	C	7.2148382024	6.8883653469	14.0283430912
C	-0.2469024286	5.4420718307	14.0354477336	C	5.9908935310	7.6100418501	14.1266179645
C	-0.2466656561	6.8768329360	14.0166535168	C	5.9772451376	9.0244142624	14.0887646304
C	-1.4889564094	7.5967730894	14.0236319439	C	4.7203976299	9.7502167917	14.0991410555
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C	-2.7297435444	9.7505102580	14.0417766506	C	3.4871507194	11.9068214717	14.0273299670
C	-2.7300921708	11.1862948181	14.0480041266	C	3.4868398157	13.3432941813	14.0364767084
C	-3.9725026172	11.9036040823	14.0535447218	C	2.2429925331	14.0599564970	14.0392542604
C	-3.9733494218	13.3388799278	14.0514209219	C	10.9446939579	0.4211865771	14.0476561633
C	-5.2168943854	14.0563293233	14.0522602269	C	9.7011075584	1.1383703690	14.0439416455
C	3.4857883499	0.4173014894	14.0451233528	C	12.1867500663	2.5742997070	14.0530279081
C	2.2423004923	1.1371199610	14.0433933926	C	10.9446171408	3.2915184547	14.0470170387
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C	3.4952767133	4.7266692964	14.1008969380	C	9.7039052634	6.8814404607	14.0120390939
C	2.2373372319	5.4502026696	14.1107158956	C	8.4620581322	7.6021840669	13.9959809582
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C	0.9972955580	7.5929375414	14.0327666415	C	7.2171961554	9.7506868081	14.0303681562
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C	-0.2411049222	9.7493198349	14.0246801918	C	5.9705315709	11.9048355997	14.0404148948
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C	4.7278902670	1.1329932382	14.0323222968	C	13.4304736600	3.2910726619	14.0530986753
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C	0.9994899924	11.9060021603	14.0182634688	C	7.2152547627	14.0579811368	14.0494587134
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C	-0.2436117161	14.0580298392	14.0417372202	C	14.6737498574	1.1381825178	14.0556198258
C	8.4582851728	0.4195716130	14.0401680059	C	-0.2448660989	2.5731292853	14.0471317477
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C	-1.4904052152	4.7237852937	14.0391814005	Ni	-3.7806301286	10.6572971443	11.9762246425
C	-2.7328221960	5.4428677885	14.0402578891	Ni	-5.0164038560	9.9452643480	10.0000000000
C	-2.7319863634	6.8787212374	14.0360905864	Ni	-5.0188749129	11.3673895493	13.9653378509
C	-3.9740187846	7.5972949716	14.0421795612	Ni	-5.0156508943	12.7966689081	11.9749150146
C	-3.9731481325	9.0329391739	14.0445709216	Ni	-6.2521252350	12.0854874330	10.0000000000
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C	-6.4598112022	13.3393277537	14.0534182069	Ni	3.6340521219	0.6680202260	13.9617681301
C	-7.7041256227	14.0573534027	14.0519781216	Ni	3.6341925213	2.0968997909	11.9719714189
C	0.9983849672	0.4187660174	14.0485001400	Ni	2.3977843820	1.3842911590	10.0000000000
C	-0.2452589910	1.1367583494	14.0498113147	Ni	2.3960928205	2.8047909758	13.9575853767
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O	4.0362118853	9.8720544070	17.4333537632	Ni	1.1620630030	3.5245142430	10.0000000000
C	5.1814517664	7.8499476123	17.0177355204	Ni	1.1619850896	4.9533481575	13.9559840120
O	6.3230253559	8.4929968547	17.3705272403	Ni	1.1631070049	6.3812390441	11.9722201067
C	5.1585750590	6.6003424806	16.2736942906	Ni	-0.0736583760	5.6647373280	10.0000000000
H	6.1126242226	6.0675726435	16.2750104485	Ni	-0.0768687622	7.0943216532	13.9621295317
H	4.3720389768	5.9137941283	16.6021105838	Ni	-0.0713606616	8.5197264931	11.9772736319
C	2.8693058919	7.9418855217	16.4527961626	Ni	-1.3093797550	7.8049604120	10.0000000000
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C	2.7846578204	10.5495896540	17.6087946412	Ni	-2.5451011340	9.9451834970	10.0000000000
C	7.5108666500	7.7041713814	17.5457170880	Ni	-2.5463795015	11.3692879043	13.9655422294
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TS-G/Ni-MAH				Ni	6.1066056827	2.0980126675	11.9751338292
Ni	1.1613214687	0.6696420820	13.9635385266	Ni	4.8690871040	1.3842103070	10.0000000000
Ni	1.1615230470	2.0971985715	11.9733492966	Ni	4.8708235783	2.8087555103	13.9560587593
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TS-G/Ni-DMBD				Ni	6.1017502868	2.0993145119	11.9705749880
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C	3.1850713826	8.0450541785	18.2695554677	C	4.565837138	6.853034709	13.859997019
H	2.2560241778	8.6238438327	18.2816084426	C	3.371517000	7.542555974	13.855759289
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C	2.9854942091	10.6623298620	19.5063426999	C	2.142117344	9.708224225	14.183583235
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H	3.2071553810	11.6589338706	19.9032440514	C	0.911150707	11.838789161	14.119794425
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H	8.1512177487	7.5669312828	18.6509966066	C	7.062833992	1.185224815	14.071525783
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Cu	9.724557177	8.338553264	6.750759000	C	2.189445085	1.234955831	14.022254949
Cu	8.482071898	11.930503117	10.953578658	C	4.673975249	2.669520100	14.003712715
Cu	9.726689617	11.208063082	8.859518089	C	3.429458478	3.381577073	13.960451306
Cu	8.481439833	10.492047035	6.750759000	C	3.425709240	4.815278626	13.892024231
Cu	7.236786366	14.088019507	10.955710865	C	2.181714284	5.533401137	13.891153275
Cu	8.479400218	13.364333841	8.857436145	C	2.177795146	6.967284406	13.893615474
Cu	7.238322489	12.645540806	6.750759000	C	0.942781527	7.691862699	14.003781616
Cu	14.692867285	1.163853814	10.964185198	C	0.962948236	9.134786563	14.083706926
Cu	15.936996510	0.446555008	8.857851202	C	-0.287628874	9.849772021	14.073540362
Cu	5.995205145	14.799034577	6.750759000	C	-0.290938450	11.283970348	14.093049432
Cu	-1.468750333	3.317345248	10.963937114	C	-1.536491429	12.002651099	14.092063833
Cu	-0.225229863	2.598810982	8.857947150	C	-1.536578988	13.437374570	14.084846930
Cu	15.940282899	1.878152198	6.750759000	C	-2.779636746	14.157034946	14.072944084
Cu	-2.709053790	5.470536046	10.971121141	C	5.920710444	0.517189320	14.060918140
Cu	-1.466365957	4.752969912	8.860202128	C	4.676934600	1.235488789	14.036451027
Cu	14.697165555	4.031645969	6.750759000	C	7.161167170	2.672668396	14.057035793
Cu	-3.949930597	7.622785707	10.973582607	C	5.917279697	3.393556841	14.022646231
Cu	-2.706502309	6.904940501	8.864160098	C	5.914449123	4.821538982	14.007638756
Cu	13.454048211	6.185139740	6.750759000	C	4.669311985	5.529146333	13.896558181
Cu	-5.192368926	9.774878947	10.973878342	C	4.638270775	6.955473039	13.876431541
Cu	-3.948723250	9.056345830	8.864756444	C	3.429087944	7.655340973	13.869565918
Cu	12.210930867	8.338633511	6.750759000	C	3.506234875	9.093713210	14.331473253
Cu	-6.437953072	11.929076987	10.966330448	C	2.194532263	9.848278799	14.159760068
Cu	-5.192156259	11.209623628	8.863154638	C	2.196674788	11.272059661	14.097812804
Cu	10.967813524	10.492127282	6.750759000	C	0.951922173	11.999305385	14.084062797
Cu	-7.682147843	14.084471042	10.961273466	C	0.950513595	13.437788066	14.075586887
Cu	-6.437712270	13.363660104	8.861418899	C	-0.293287527	14.155741756	14.080120863
Cu	9.724696180	12.645621053	6.750759000	C	8.405768694	0.518578215	14.074569181
Cu	-0.224973857	1.163998842	10.961440945	C	7.162646829	1.237718923	14.066922190
Cu	1.019611232	0.444390934	8.858373474	C	9.644188793	2.676851519	14.079386873
Cu	8.481578836	14.799114825	6.750759000	C	8.400614050	3.395798894	14.068581178
C	2.186686558	2.668262266	13.988945791	C	8.398391702	4.834422582	14.080703116
C	0.942679945	3.386311884	13.988918543	C	7.153735310	5.560213513	14.092788182

C	7.156523323	6.983201754	14.170581117	C	-4.024180529	9.133052677	14.076055083
C	5.846333617	7.742579346	14.335310116	C	-5.268111124	9.851126388	14.075703554
C	5.923051813	9.178407507	13.855301900	C	-5.265446928	11.287047545	14.067879317
C	4.709816646	9.876750592	13.845546167	C	-6.508831926	12.005409620	14.045055211
C	4.681941917	11.303487874	13.897197736	C	-6.509298151	13.441076043	14.038302809
C	3.437993011	12.010718615	14.027076366	C	-7.752369414	14.161072863	14.025769911
C	3.434771245	13.440729868	14.038014150	C	0.946876372	0.520209111	14.028332819
C	2.190643472	14.161255637	14.069332950	C	-0.297133349	1.238481206	14.028453286
C	10.890636720	0.521494084	14.075065358	C	5.095876601	6.847354059	16.710151277
C	9.646805320	1.239584922	14.077288846	C	5.376812916	8.093396738	15.904287728
C	12.131796462	2.676069126	14.076224139	C	4.038780786	8.867371100	15.901098396
C	10.888044697	3.394207010	14.088308024	C	3.098142641	8.005350305	16.709021978
C	10.887561263	4.829163553	14.096767182	H	6.208444902	8.644776231	16.360227690
C	9.642241343	5.548583023	14.100871495	H	4.102162113	9.864409852	16.354577128
C	9.640145353	6.982676732	14.090830871	O	5.854205143	5.969935419	17.030463151
C	8.387858165	7.697459213	14.106556271	O	1.960382954	8.227371770	17.031390876
C	8.406737587	9.141490491	14.030440717	O	3.738914774	6.808174214	17.071161110
C	7.171821223	9.865510849	13.901241725	FS-G/Cu-DMBD			
C	7.170336615	11.300918261	13.893908568	Cu	1.023907896	3.315598239	10.970272288
C	5.925760492	12.019716219	13.893019084	Cu	2.265605905	2.595061643	8.860255593
C	5.922599373	13.452955444	13.967059728	Cu	1.022195002	1.877689897	6.750759000
C	4.677867420	14.164737096	14.015286772	Cu	-0.221309574	5.466103697	10.966880487
C	13.376673280	0.523938288	14.044167015	Cu	1.028415817	4.752599630	8.867557723
C	12.133107050	1.241475460	14.068788187	Cu	-0.220992195	4.031141533	6.750759000
C	14.618611403	2.675630273	14.050163382	Cu	-1.465515175	7.619243556	10.959770086
C	13.374685645	3.393731108	14.068144241	Cu	-0.217201557	6.903397358	8.863286379
C	13.375002001	4.829283071	14.074357687	Cu	-1.464179392	6.184593169	6.750759000
C	12.130176615	5.546394530	14.088464438	Cu	-2.708360379	9.772441987	10.962445844
C	12.130268462	6.982404681	14.082981437	Cu	-1.465973662	9.055271062	8.858455445
C	10.886397556	7.700670791	14.080525111	Cu	-2.707366589	8.338044805	6.750759000
C	10.892892843	9.136324508	14.071525403	Cu	-3.951255854	11.926025302	10.968393541
C	9.646959586	9.853682652	14.041186224	Cu	-2.709132313	11.209026178	8.861229808
C	9.652652838	11.292058896	14.016532596	Cu	-3.950553786	10.491496441	6.750759000
C	8.413382264	12.014250714	13.968200330	Cu	-5.195381879	14.078862729	10.967224776
C	8.409633718	13.447609858	13.995898160	Cu	-3.951132107	13.362410628	8.862135808
C	7.165840358	14.166032060	13.995812690	Cu	-5.193740982	12.644948077	6.750759000
C	15.864947429	0.524835988	14.024763940	Cu	2.262143816	1.158108392	10.963219815
C	14.619920047	1.241037654	14.038581126	Cu	3.507095314	0.440096447	8.860887260
C	-0.299585057	2.672026914	14.021188038	Cu	-6.436928179	14.798399713	6.750759000
C	-1.542892735	3.390908572	14.035750256	Cu	3.506377578	3.312922018	10.969673859
C	-1.542952809	4.826310870	14.035779630	Cu	4.749885205	2.593796785	8.859295105
C	-2.786663465	5.544418387	14.061868692	Cu	3.508822716	1.877836171	6.750759000
C	-2.784013000	6.980499442	14.066237860	Cu	2.266148112	5.471194839	10.991744049
C	-4.028223169	7.697875016	14.075780103	Cu	3.511804242	4.752565211	8.879425306

Cu	2.265635519	4.031287807	6.750759000	Cu	7.228378965	6.908538452	8.875311968
Cu	1.022780480	7.621251424	10.979722083	Cu	5.995703749	6.185031989	6.750759000
Cu	2.271416339	6.905175859	8.881377504	Cu	4.747458829	9.770079319	10.987074619
Cu	1.022448322	6.184739443	6.750759000	Cu	5.994120300	9.050198380	8.879508203
Cu	-0.222455659	9.773509082	10.964884160	Cu	4.752516552	8.338483625	6.750759000
Cu	1.022200002	9.054755733	8.865635128	Cu	3.508608556	11.926257644	10.965801749
Cu	-0.220738875	8.338191078	6.750759000	Cu	4.752541099	11.201875205	8.866520230
Cu	-1.463973115	11.926631387	10.962229643	Cu	3.509329356	10.491935261	6.750759000
Cu	-0.222001548	11.209107580	8.858319624	Cu	2.266493508	14.081329443	10.961796587
Cu	-1.463926072	10.491642714	6.750759000	Cu	3.509623852	13.359763419	8.859832804
Cu	-2.707271318	14.078550882	10.964338390	Cu	2.266142159	12.645386897	6.750759000
Cu	-1.463528851	13.363304023	8.858613532	Cu	9.725513725	1.161011636	10.961266544
Cu	-2.707113269	12.645094350	6.750759000	Cu	10.969478996	0.443610718	8.859831285
Cu	4.751009396	1.158281512	10.963306244	Cu	1.022954962	14.798838533	6.750759000
Cu	5.995418377	0.441962374	8.859081346	Cu	10.966400374	3.313504113	10.963780059
Cu	-3.950300466	14.798545986	6.750759000	Cu	12.210412873	2.596981701	8.861190195
Cu	5.990781678	3.313496054	10.962925333	Cu	10.968705857	1.878274991	6.750759000
Cu	7.235754455	2.599215407	8.859125323	Cu	9.721496679	5.467374254	10.963542358
Cu	5.995450429	1.877982444	6.750759000	Cu	10.964966177	4.750049470	8.859629249
Cu	4.746655129	5.472922034	11.045684481	Cu	9.725518660	4.031726627	6.750759000
Cu	5.984607355	4.755498741	8.875415858	Cu	8.478576176	7.622844296	10.961995189
Cu	4.752263232	4.031434080	6.750759000	Cu	9.721440994	6.903264689	8.858894999
Cu	3.502578761	7.622862171	11.063058896	Cu	8.482331463	6.185178263	6.750759000
Cu	4.748935848	6.903742155	8.907660439	Cu	7.236294341	9.774190212	10.969067280
Cu	3.509076035	6.184885716	6.750759000	Cu	8.483032249	9.058303933	8.859081843
Cu	2.263809516	9.771246988	10.977216684	Cu	7.239144266	8.338629899	6.750759000
Cu	3.509185652	9.047615348	8.880505096	Cu	5.993073415	11.922593821	10.970010944
Cu	2.265888839	8.338337352	6.750759000	Cu	7.239571316	11.208785649	8.860249938
Cu	1.022390575	11.927187247	10.958291549	Cu	5.995957069	10.492081535	6.750759000
Cu	2.266792497	11.204287171	8.862510119	Cu	4.752296895	14.079866181	10.963496512
Cu	1.022701642	10.491788988	6.750759000	Cu	5.994623530	13.360113958	8.861807343
Cu	-0.220046434	14.080924783	10.961436997	Cu	4.752769872	12.645533171	6.750759000
Cu	1.024394990	13.362634412	8.858314217	Cu	12.211327572	1.159780872	10.968248683
Cu	-0.220485555	12.645240624	6.750759000	Cu	13.454192983	0.442315983	8.861902147
Cu	7.238363701	1.159606547	10.958785859	Cu	3.509582676	14.798984807	6.750759000
Cu	8.483028180	0.443752526	8.857641701	Cu	13.453868241	3.312330139	10.968191066
Cu	-1.463672752	14.798692260	6.750759000	Cu	14.698221561	2.597050606	8.862094327
Cu	8.478921985	3.314769445	10.964044497	Cu	13.455333571	1.878421264	6.750759000
Cu	9.722770074	2.598929965	8.859491268	Cu	12.209686840	5.465025845	10.961863606
Cu	8.482078143	1.878128718	6.750759000	Cu	13.454662586	4.747991928	8.860271957
Cu	7.234401383	5.468092213	10.966652801	Cu	12.212146374	4.031872900	6.750759000
Cu	8.474619020	4.753767615	8.860199149	Cu	10.967295693	7.619717559	10.958499578
Cu	7.238890946	4.031580353	6.750759000	Cu	12.211371917	6.900452429	8.857742868
Cu	5.985189853	7.619611397	11.044066444	Cu	10.968959177	6.185324536	6.750759000

Cu	9.724716100	9.774081030	10.962601045	C	-5.223243056	14.061514012	14.059919584
Cu	10.969064141	9.055216896	8.858799059	C	3.479126834	0.421933512	14.045146414
Cu	9.725771980	8.338776172	6.750759000	C	2.236202453	1.142406874	14.038711414
Cu	8.480258777	11.928847853	10.962837906	C	4.722044787	2.574352469	14.014619507
Cu	9.726491947	11.211136488	8.860649265	C	3.481016785	3.295244140	14.031664594
Cu	8.482584783	10.492227808	6.750759000	C	3.490852141	4.731888982	14.102030138
Cu	7.236818454	14.079653479	10.965021540	C	2.230290221	5.459107801	14.102703293
Cu	8.481315741	13.364503083	8.859428966	C	2.217759944	6.873848687	14.140945427
Cu	7.239397586	12.645679444	6.750759000	C	0.991956827	7.595268317	14.029732074
Cu	14.697238918	1.159216192	10.969360609	C	0.991243853	9.040292315	14.027662839
Cu	15.939680953	0.443597530	8.861230202	C	-0.245224877	9.754171464	14.011424395
Cu	5.996210389	14.799131080	6.750759000	C	-0.249329529	11.193734127	14.007207239
Cu	-1.465216437	3.311611819	10.963787310	C	-1.492517197	11.909126672	14.029415117
Cu	-0.219565913	2.597834106	8.861760246	C	-1.492970013	13.344620099	14.032605398
Cu	15.941961284	1.878567538	6.750759000	C	-2.736483383	14.061328621	14.041968213
Cu	-2.709375202	5.464527802	10.962269753	C	5.965494640	0.422139599	14.026580614
Cu	-1.461713626	4.750055735	8.860173903	C	4.721627857	1.137530194	14.025497108
Cu	14.698774087	4.032019174	6.750759000	C	7.209218372	2.576827256	14.004221674
Cu	-3.952547424	7.618227460	10.961717393	C	5.964050737	3.292015673	13.996531480
Cu	-2.707195466	6.900032811	8.858576039	C	5.959275447	4.728233543	14.031309044
Cu	13.455586891	6.185470810	6.750759000	C	4.721913192	5.429530036	14.141685804
Cu	-5.194292258	9.772722344	10.964388316	C	4.789548049	6.851796975	14.662658623
Cu	-3.951892791	9.053566471	8.858770866	C	3.416204189	7.643845475	14.661081006
Cu	12.212399694	8.338922446	6.750759000	C	3.480417497	9.060787555	14.117735648
Cu	-6.438481930	11.926647867	10.967200700	C	2.243888708	9.761041475	14.011023977
Cu	-5.194834907	11.208017142	8.862052243	C	2.238495953	11.197482350	13.978392616
Cu	10.969212497	10.492374082	6.750759000	C	0.993401901	11.912520143	13.996392532
Cu	-7.682152207	14.079206718	10.968272354	C	0.993856025	13.347693119	14.016396522
Cu	-6.438525368	13.362523742	8.861293849	C	-0.249742570	14.063755926	14.025891908
Cu	9.726025300	12.645825718	6.750759000	C	8.452222720	0.425199664	14.026737390
Cu	-0.222931085	1.159399366	10.964870616	C	7.208722973	1.141472485	14.019916266
Cu	1.019876191	0.441800229	8.859590643	C	9.694904498	2.579725790	14.031191868
Cu	8.482838103	14.799277353	6.750759000	C	8.451901026	3.295250604	14.013005949
C	2.236711180	2.576989240	14.026363065	C	8.447796395	4.735092306	14.014278126
C	0.990875094	3.296297327	14.025323832	C	7.211705557	5.449134539	14.031331356
C	0.991006035	4.733183834	14.029379986	C	7.209729968	6.894083757	14.011419508
C	-0.253922900	5.447447169	14.012609668	C	5.984206640	7.614667098	14.116211330
C	-0.254332763	6.881926468	13.993943899	C	5.971313319	9.028381116	14.077442364
C	-1.496154109	7.602632265	14.003208067	C	4.711504654	9.755497480	14.078857543
C	-1.494430805	9.038120817	14.010468881	C	4.721417268	11.191518328	14.015866121
C	-2.735933142	9.756285522	14.029634906	C	3.481059137	11.912909621	14.001724580
C	-2.736963126	11.192280348	14.042856752	C	3.480858073	13.349852907	14.020654988
C	-3.978986069	11.909355515	14.056502481	C	2.237380932	14.066137394	14.025743680
C	-3.979998931	13.344327925	14.055427385	C	10.938909701	0.427316566	14.042591124

C	9.695495783	1.144097092	14.034847041	O	4.024917276	9.884679886	17.385046711
C	12.180829402	2.579751596	14.057095777	C	5.263347191	7.905977815	16.966259181
C	10.939045518	3.296832389	14.044745191	O	6.416417826	8.507303801	17.388140380
C	10.937614413	4.732784949	14.030295112	C	5.229020862	6.619647651	16.228886375
C	9.696551603	5.451849290	14.010304848	H	6.194808958	6.108436552	16.228736209
C	9.697668525	6.887170643	13.999303604	H	4.492559545	5.921053767	16.649766507
C	8.456040058	7.608356661	13.981313421	C	2.991455908	7.908171215	16.227951471
C	8.454390816	9.042322218	14.002650069	H	2.062616346	8.483767829	16.226300672
C	7.209557558	9.755503131	14.016468295	H	2.760147383	6.920313200	16.649299712
C	7.210167725	11.191755529	14.018824687	C	2.726230315	10.451917760	17.596519962
C	5.964749059	11.910505677	14.019175394	C	7.560133681	7.671486741	17.602214737
C	5.965469309	13.344724449	14.035467826	H	2.900794350	11.423258636	18.072528631
C	4.722729067	14.065713759	14.044921173	H	2.117599018	9.818282526	18.261308968
C	13.425216153	0.426358595	14.060844776	H	2.192473078	10.605547680	16.644649551
C	12.182268241	1.144513061	14.056937191	H	8.309734286	8.313395889	18.078235943
C	14.667291977	2.578259435	14.059251670	H	7.963331799	7.287368525	16.651140770
C	13.424325152	3.296247301	14.056489975	H	7.318798253	6.827212769	18.267901333
C	13.423830238	4.731429199	14.040827291	FS-G/Ni-MAH			
C	12.181333435	5.449933087	14.033447332	Ni	1.160043908	0.671987754	13.964308820
C	12.182496579	6.885704628	14.026502194	Ni	1.161034944	2.097745107	11.974137333
C	10.940650961	7.605095518	14.018738832	Ni	-0.072797328	1.383845683	10.000000000
C	10.941152654	9.041090387	14.025025063	Ni	-0.073143056	2.811486558	13.963270480
C	9.699045686	9.760059088	14.021166580	Ni	-0.072173061	4.239064188	11.974517636
C	9.698048848	11.193484654	14.043758378	Ni	-1.306423424	3.522722745	10.000000000
C	8.452130571	11.908967364	14.036286600	Ni	-1.305818408	4.951870299	13.964864881
C	8.452871846	13.345191716	14.045528429	Ni	-1.304003336	6.377781464	11.975570087
C	7.209359420	14.063175803	14.045682798	Ni	-2.540049520	5.661599807	10.000000000
C	15.911850523	0.424919978	14.054564662	Ni	-2.541700280	7.087955035	13.963934466
C	14.667988137	1.143525234	14.063612912	Ni	-2.539024392	8.515196817	11.975870961
C	-0.250961161	2.578073304	14.037092841	Ni	-3.773675616	7.800476868	10.000000000
C	-1.496446929	3.294249619	14.044446932	Ni	-3.775453042	9.226152711	13.965883896
C	-1.497628245	4.728077242	14.023771683	Ni	-3.772032877	10.652674553	11.976352027
C	-2.739289938	5.447342356	14.025799088	Ni	-5.007301712	9.939353930	10.000000000
C	-2.738496095	6.883717937	14.018810180	Ni	-5.008638858	11.362808598	13.965455052
C	-3.980605977	7.602451721	14.027066662	Ni	-5.005278548	12.791112937	11.975147914
C	-3.979528850	9.038607494	14.032946269	Ni	-6.240927808	12.078230992	10.000000000
C	-5.222161547	9.757326217	14.041457153	Ni	-6.239899632	13.504422975	13.962119035
C	-5.222570273	11.192678717	14.054948553	Ni	-6.239720512	14.931000481	11.974385863
C	-6.465928194	11.910013395	14.059737425	Ni	-7.474553904	14.217108054	10.000000000
C	-6.466057885	13.344533063	14.062703035	Ni	3.631230495	0.671433289	13.962594013
C	-7.709998297	14.062197247	14.054876879	Ni	3.631668569	2.098531697	11.972785495
C	0.992481745	0.423671468	14.046164031	Ni	2.396345600	1.384937289	10.000000000
C	-0.251013936	1.141677001	14.046612413	Ni	2.395146714	2.805842863	13.958255142
C	4.085061191	8.584671931	16.965615447	Ni	2.395492227	4.236833319	11.966761514

Ni	1.162719504	3.523814351	10.000000000	Ni	6.103818606	6.383801844	11.986082515
Ni	1.164517463	4.955612282	13.956141619	Ni	4.867379265	5.664874625	10.000000000
Ni	1.165906966	6.382106732	11.973874765	Ni	4.874054674	7.104918917	13.952730652
Ni	-0.070906592	5.662691413	10.000000000	Ni	4.862674053	8.520024506	11.964945380
Ni	-0.072994003	7.095034241	13.965136624	Ni	3.633753169	7.803751687	10.000000000
Ni	-0.065425327	8.518616001	11.980360575	Ni	3.649397776	9.229189870	13.997436599
Ni	-1.304532688	7.801568475	10.000000000	Ni	3.630229504	10.651581425	11.978406718
Ni	-1.301280871	9.229264329	13.965845787	Ni	2.400127073	9.942628749	10.000000000
Ni	-1.301820510	10.655449693	11.976996393	Ni	2.401650710	11.360786019	13.983163601
Ni	-2.538158784	9.940445537	10.000000000	Ni	2.400336041	12.791287762	11.981436841
Ni	-2.538195219	11.365871710	13.965283918	Ni	1.166500977	12.081505811	10.000000000
Ni	-2.536061848	12.792985694	11.975702150	Ni	1.170319832	13.503469134	13.970937289
Ni	-3.771784880	12.079322598	10.000000000	Ni	1.166827245	14.933757289	11.976848005
Ni	-3.770893161	13.505592021	13.963425600	Ni	-0.067125119	14.220382873	10.000000000
Ni	-3.769348349	14.931818335	11.975188696	Ni	11.037459989	0.677642097	13.964471228
Ni	-5.005410976	14.218199660	10.000000000	Ni	11.037091538	2.102690044	11.973860719
Ni	6.101932901	0.675164887	13.964825988	Ni	9.803774385	1.388212108	10.000000000
Ni	6.101953249	2.100860966	11.976417089	Ni	9.802925522	2.815658856	13.964300983
Ni	4.865488528	1.386028896	10.000000000	Ni	9.802867068	4.241876046	11.975714894
Ni	4.868472123	2.811332555	13.958287218	Ni	8.570148289	3.527089170	10.000000000
Ni	4.870916095	4.239873777	11.969719595	Ni	8.571456008	4.956966772	13.974486944
Ni	3.631862432	3.524905957	10.000000000	Ni	8.568893574	6.381047265	11.987992204
Ni	3.627220570	4.943446199	13.932825087	Ni	7.336522193	5.665966232	10.000000000
Ni	3.632308170	6.380311156	11.958411968	Ni	7.335883545	7.091228957	14.017360288
Ni	2.398236336	5.663783019	10.000000000	Ni	7.334575392	8.512949321	11.985850396
Ni	2.402813211	7.111421786	13.947440056	Ni	6.102896097	7.804843294	10.000000000
Ni	2.401824260	8.525318992	11.979926924	Ni	6.098187329	9.216937643	13.947425964
Ni	1.164610240	7.802660081	10.000000000	Ni	6.101919065	10.656420054	11.958077241
Ni	1.174542418	9.234750708	13.991124105	Ni	4.869270001	9.943720355	10.000000000
Ni	1.167382451	10.653089042	11.984628821	Ni	4.855262669	11.357797833	13.953119222
Ni	-0.069015856	9.941537143	10.000000000	Ni	4.866973668	12.791809776	11.976483074
Ni	-0.066305060	11.366920767	13.973637278	Ni	3.635643905	12.082597417	10.000000000
Ni	-0.067387688	12.792412587	11.978414977	Ni	3.629533443	13.510050060	13.965558519
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Ni	-2.536268048	14.219291266	10.000000000	Ni	13.506674476	2.103055629	11.974914205
Ni	8.569466605	0.675520162	13.966651927	Ni	12.272917313	1.389303714	10.000000000
Ni	8.567398992	2.102683202	11.976568622	Ni	12.272115731	2.817397544	13.962315600
Ni	7.334631457	1.387120502	10.000000000	Ni	12.273174559	4.242521034	11.973659162
Ni	7.331994905	2.822129553	13.970348728	Ni	11.039291217	3.528180776	10.000000000
Ni	7.334210112	4.245292638	11.981785938	Ni	11.037986626	4.956501649	13.963388603
Ni	6.101005361	3.525997564	10.000000000	Ni	11.038793793	6.381897600	11.975288188
Ni	6.098319629	4.969800640	13.978799213	Ni	9.805665121	5.667057838	10.000000000

Ni	9.804283442	7.092705090	13.975159282	C	-6.237810514	12.077343069	16.106568956
Ni	9.801355704	8.518461825	11.983270864	C	-6.237404933	13.503697442	16.104582009
Ni	8.572039025	7.805934900	10.000000000	C	-7.471861223	14.217135697	16.111544294
Ni	8.555597192	9.225488212	13.980072974	C	3.633116193	0.670734370	16.106473245
Ni	8.574178650	10.654374656	11.970204836	C	2.397988277	1.382992307	16.113180182
Ni	7.338412929	9.944811962	10.000000000	C	2.396929863	2.808355482	16.101417787
Ni	7.343616594	11.378529758	13.933870630	C	1.162209577	3.520920483	16.104987531
Ni	7.338614725	12.799882885	11.967140800	C	1.161494121	4.946269971	16.085551871
Ni	6.104786833	12.083689023	10.000000000	C	-0.071278785	5.661004276	16.098401877
Ni	6.099143388	13.505168435	13.959329452	C	-0.067980675	7.087856442	16.111528576
Ni	6.103420884	14.935277967	11.974880504	C	-1.303171792	7.799466212	16.119620858
Ni	4.871160737	14.222566085	10.000000000	C	-1.293857499	9.224668554	16.103549856
Ni	15.973911941	0.677647760	13.963444283	C	-2.531003428	9.937881578	16.098826171
Ni	15.976387660	2.104377091	11.974741427	C	-2.530857380	11.364491935	16.101574095
Ni	14.742060242	1.390395321	10.000000000	C	-3.766698363	12.077073161	16.104778044
Ni	14.742436333	2.816853983	13.963122407	C	-3.766613104	13.503463639	16.105439250
Ni	14.743009101	4.244139797	11.975007801	C	-5.001535206	14.216370186	16.105790617
Ni	13.508434146	3.529272382	10.000000000	C	6.102774355	0.671251885	16.110270065
Ni	13.507604638	4.956296556	13.962537499	C	4.868212575	1.384090362	16.107987902
Ni	13.508840722	6.382921526	11.974024085	C	4.866943010	2.810698558	16.099308334
Ni	12.274808050	5.668149444	10.000000000	C	3.632059193	3.520320783	16.082105220
Ni	12.273721411	7.095332362	13.964709913	C	3.631419900	4.945827693	16.029538785
Ni	12.273197423	8.521678855	11.976768790	C	2.396237394	5.658467127	16.031756574
Ni	11.041181954	7.807026506	10.000000000	C	2.395513098	7.083432822	16.005636917
Ni	11.031247330	9.231397924	13.972848114	C	1.165498555	7.798536633	16.098711847
Ni	11.041983640	10.657725132	11.977286234	C	1.189703929	9.225626832	16.155159651
Ni	9.807555858	9.945903568	10.000000000	C	-0.052361845	9.935704508	16.115572919
Ni	9.808911026	11.370030247	13.959430544	C	-0.057422192	11.362074691	16.121576288
Ni	9.809122614	12.798347009	11.972396676	C	-1.293871311	12.075716367	16.107754116
Ni	8.573929762	12.084780630	10.000000000	C	-1.296299011	13.502502213	16.104716387
Ni	8.577305024	13.515126835	13.957749448	C	-2.531223729	14.216593583	16.106650759
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H 6.372006876 8.727748183 18.531641231
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O 5.999840293 6.016721788 19.100064607
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FS-G/Ni-DMBD
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Ni 1.164553777 2.101469555 11.972461303
Ni -0.073444473 1.384451149 10.000000000
Ni -0.073820053 2.810624548 13.958671318
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Ni -1.307909517 4.951186835 13.958479932
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Ni	-5.015802962	14.226214324	10.000000000	Ni	11.046791918	2.097341380	11.974157834
Ni	6.103979839	0.669342124	13.959100077	Ni	9.811808410	1.384657951	10.000000000
Ni	6.102976217	2.100104987	11.970063235	Ni	9.812568848	2.810715357	13.962422750
Ni	4.869181969	1.384554550	10.000000000	Ni	9.811873126	4.238061140	11.972626535
Ni	4.869131992	2.812980050	13.956618710	Ni	8.576196459	3.524943197	10.000000000
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Ni	3.633570017	3.524839796	10.000000000	Ni	8.573131711	6.379574059	11.968887043
Ni	3.643160847	4.978322540	14.006507402	Ni	7.340584507	5.665228443	10.000000000
Ni	3.639021284	6.387222553	12.013160983	Ni	7.339186648	7.085426215	13.952248802
Ni	2.397958065	5.665125042	10.000000000	Ni	7.331194073	8.519496437	11.972987194
Ni	2.427639465	7.094297400	14.039765372	Ni	6.104972555	7.805513688	10.000000000
Ni	2.408533573	8.511556886	11.991756040	Ni	6.087639459	9.212306788	13.999398951
Ni	1.162346114	7.805410287	10.000000000	Ni	6.100278212	10.647293959	11.981164793
Ni	1.181017764	9.221131289	13.964507491	Ni	4.869360604	9.945798934	10.000000000
Ni	1.165168820	10.653398955	11.969477685	Ni	4.869995687	11.371533121	13.958843821
Ni	-0.073265838	9.945695533	10.000000000	Ni	4.868896021	12.794147797	11.972542490
Ni	-0.073554528	11.369476532	13.955657176	Ni	3.633748652	12.086084180	10.000000000
Ni	-0.071893602	12.797525342	11.972762650	Ni	3.634702609	13.511834063	13.959153118
Ni	-1.308877790	12.085980779	10.000000000	Ni	3.633724037	14.938021221	11.974354017
Ni	-1.309002609	13.512417151	13.961815320	Ni	2.398136700	14.226369426	10.000000000
Ni	-1.308735157	14.939981463	11.973472290	Ni	13.518192114	0.671009540	13.962641954
Ni	-2.544489741	14.226266025	10.000000000	Ni	13.518881406	2.097514072	11.973439301
Ni	8.576606113	0.670361339	13.963632812	Ni	12.283121631	1.384709651	10.000000000
Ni	8.575869014	2.097759149	11.972850099	Ni	12.282970006	2.811472982	13.961683959
Ni	7.340495189	1.384606250	10.000000000	Ni	12.283180604	4.238699040	11.973800222
Ni	7.340467069	2.808931795	13.954996815	Ni	11.047509679	3.524994897	10.000000000
Ni	7.336878501	4.240427756	11.971259483	Ni	11.048162244	4.951894903	13.962077179
Ni	6.104883238	3.524891496	10.000000000	Ni	11.047650852	6.378756163	11.972224476
Ni	6.108635525	4.955807755	13.961401740	Ni	9.811897728	5.665280143	10.000000000
Ni	6.099542434	6.380618551	11.972761000	Ni	9.814202299	7.093531344	13.952724022
Ni	4.869271286	5.665176742	10.000000000	Ni	9.809395295	8.519643270	11.969415399
Ni	4.899810501	7.078200002	14.044369161	Ni	8.576285776	7.805565389	10.000000000
Ni	4.864862249	8.509727614	12.007782284	Ni	8.575938476	9.231768150	13.954719123
Ni	3.633659334	7.805461988	10.000000000	Ni	8.573220680	10.657325460	11.973214352
Ni	3.645347806	9.203088563	14.034448293	Ni	7.340673824	9.945850635	10.000000000
Ni	3.636093724	10.644690696	11.980727803	Ni	7.337136009	11.364624791	13.962032921
Ni	2.398047383	9.945747234	10.000000000	Ni	7.338494400	12.795339489	11.973637346
Ni	2.400960293	11.370500505	13.946648316	Ni	6.105061873	12.086135880	10.000000000

Ni	6.105816229	13.512742967	13.960502972	C	-0.072601721	7.090351597	16.052189869
Ni	6.104579402	14.937802126	11.973965761	C	-1.308912012	7.807102828	16.079601925
Ni	4.869449921	14.226421126	10.000000000	C	-1.308242330	9.233159245	16.099920069
Ni	15.989435681	0.671362715	13.962726308	C	-2.544056054	9.946999916	16.115200785
Ni	15.990832525	2.098679883	11.973039376	C	-2.543926789	11.373548510	16.113981150
Ni	14.754434852	1.384761352	10.000000000	C	-3.780694620	12.086499936	16.108505956
Ni	14.753761515	2.812103165	13.961686646	C	-3.781077215	13.513668570	16.104902809
Ni	14.755578835	4.239081693	11.973373634	C	-5.017220781	14.226968540	16.106571974
Ni	13.518822900	3.525046598	10.000000000	C	6.102903275	0.672783345	16.099483993
Ni	13.518941795	4.952648230	13.962719671	C	4.866842040	1.385678969	16.097581254
Ni	13.520816488	6.379156691	11.973955766	C	4.865572104	2.812702438	16.081817860
Ni	12.283210948	5.665331843	10.000000000	C	3.631185029	3.529841784	16.087764123
Ni	12.284149066	7.092498409	13.963305560	C	3.633486688	4.956624493	16.123063087
Ni	12.283071137	8.518808687	11.973651356	C	2.394976719	5.673594546	16.123221133
Ni	11.047598997	7.805617089	10.000000000	C	2.421438670	7.095824610	16.117774601
Ni	11.048987436	9.234486522	13.958891995	C	1.173706587	7.797936446	16.030241988
Ni	11.046585826	10.659845889	11.974237007	C	1.163242728	9.232082054	16.052775443
Ni	9.811987045	9.945902335	10.000000000	C	-0.070526807	9.945158861	16.092525817
Ni	9.810897783	11.374143917	13.961827196	C	-0.072391473	11.373060025	16.097950894
Ni	9.810458154	12.798743262	11.974460914	C	-1.308538225	12.086737988	16.113034573
Ni	8.576375093	12.086187581	10.000000000	C	-1.309412939	13.513822831	16.107719350
Ni	8.574664506	13.511317690	13.962298711	C	-2.545665072	14.227443854	16.105557880
Ni	8.576024985	14.939542548	11.974300377	C	8.573897126	0.673048115	16.105552873
Ni	7.340763142	14.226472827	10.000000000	C	7.337835713	1.387022247	16.099528466
C	1.159656688	0.671900840	16.101122334	C	7.337121513	2.815735243	16.081838008
C	-0.076147448	1.385327657	16.100991434	C	6.098218748	3.530596975	16.052755239
C	-0.076638379	2.812779980	16.096670026	C	6.090460250	4.961971138	16.048582266
C	-1.312888360	3.526470043	16.103548372	C	4.852656862	5.695343207	16.098632758
C	-1.312995322	4.952625456	16.098073443	C	4.924629492	7.064506426	16.737498939
C	-2.547985844	5.666972626	16.101179500	C	3.568872007	7.846252876	16.753823316
C	-2.546508840	7.093464334	16.099216073	C	3.642174271	9.206463068	16.093341201
C	-3.782160236	7.807295121	16.109231313	C	2.410834919	9.938824955	16.010755952
C	-3.780864210	9.233917007	16.110375464	C	2.401188447	11.372556948	16.041082262
C	-5.017717323	9.946798874	16.109199793	C	1.162516711	12.085310456	16.076390102
C	-5.017554093	11.373725054	16.107658534	C	1.161859846	13.513507964	16.099535811
C	-6.253981375	12.086983532	16.110370328	C	-0.073994153	14.226707501	16.108774737
C	-6.253260550	13.513823730	16.106705205	C	11.044475685	0.673520454	16.106859850
C	-7.489394437	14.226702872	16.105933518	C	9.808682178	1.387912536	16.108818269
C	3.631906233	0.671757258	16.102223835	C	9.807996242	2.815414796	16.109889343
C	2.395978064	1.385650166	16.099051263	C	8.572085661	3.529157033	16.101935415
C	2.394988721	2.812678152	16.093327756	C	8.569856896	4.956450853	16.093940864
C	1.159464993	3.525612307	16.091216239	C	7.334011030	5.669325996	16.063410301
C	1.160421695	4.954285976	16.085488231	C	7.323093695	7.099462436	16.025822026
C	-0.076594065	5.664707237	16.081820741	C	6.064518090	7.802355493	16.061670104

C	6.099314393	9.229042638	16.095639379	C	12.279217794	7.094746826	16.104798427
C	4.859641987	9.942735257	16.096855570	C	11.042767358	7.807927729	16.101100116
C	4.865969339	11.371382490	16.077812595	C	11.044123569	9.234471430	16.102768140
C	3.633763338	12.088373617	16.078310386	C	9.808143849	9.947660778	16.102857873
C	3.632233695	13.515086085	16.100780457	C	9.809000155	11.374024107	16.107652363
C	2.396347544	14.228132577	16.103190776	C	8.572449051	12.086020056	16.105244316
C	13.516293195	0.672690831	16.106623836	C	8.573674978	13.513290176	16.104581368
C	12.280211010	1.386627306	16.107845719	C	7.338141274	14.226542430	16.103957200
C	12.279467498	2.813949684	16.105699205	C	4.252045749	8.812011015	18.990828331
C	11.043782424	3.528077402	16.112458390	O	4.187770118	10.106921714	19.437449264
C	11.043157370	4.954950823	16.107061873	C	5.428316736	8.138323479	18.980888731
C	9.806796962	5.668282127	16.098939948	O	6.583622175	8.739802405	19.411698936
C	9.805545669	7.094178659	16.078179737	C	5.392707026	6.837396056	18.251864349
C	8.566505272	7.809616313	16.038956808	H	6.363575739	6.334488082	18.246233513
C	8.571655559	9.235603058	16.078479107	H	4.675818439	6.135883561	18.706689158
C	7.332855741	9.944451351	16.081786662	C	3.142869142	8.129137856	18.263018652
C	7.336509752	11.373379446	16.095925524	H	2.222315292	8.719944733	18.254203298
C	6.102324544	12.086245145	16.093686285	H	2.888957779	7.161751834	18.724023960
C	6.102365346	13.512889332	16.100717630	C	2.893374208	10.689895896	19.607705576
C	4.867169543	14.227875397	16.107110837	C	7.735057414	7.912129903	19.591375978
C	15.987448246	0.671836020	16.102163899	H	3.066793208	11.647776814	20.111587716
C	14.751654735	1.386471909	16.104510916	H	2.243364112	10.056758691	20.233666774
C	14.751060347	2.813544022	16.103913252	H	2.401267778	10.873433035	18.637324140
C	13.515219423	3.527357368	16.104838911	H	8.482374360	8.545354089	20.082901089
C	13.515188059	4.954380280	16.103383606	H	8.136202199	7.561353765	18.625603432
C	12.279241271	5.667883182	16.104789863	H	7.512043954	7.042882969	20.231023569